Radiation interaction with matter

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MNF – Micro Nano Facility

MAUD school 2015
Trento, Italy
Radiation – x-rays (photons), neutrons, electrons

Wave – particle duality

Planck / Einstein

$$E = h \nu$$

De Broglie

$$\lambda = \frac{h}{p}$$

x-rays

photons

electromagnetic radiation

0 rest mass

$$c = \lambda \nu$$

neutral particles

1.675e-27 kg

939.6 MeV/c2

electrons

charged particles

9.11e−31 kg

511.0 keV/c2

$$E_k = \frac{1}{2} mv^2 = \frac{p^2}{2m}$$

$$\lambda = \frac{h}{mv}$$

$$E_k = eV = \frac{1}{2} mv^2 = \frac{p^2}{2m}$$

$$\lambda = \frac{h}{\sqrt{2meV}} \frac{1}{\sqrt{1 + \frac{eV}{2mc^2}}}$$
Radiation – x-rays (photons), neutrons, electrons

<table>
<thead>
<tr>
<th>Interaction type</th>
<th>Interaction partners</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>x-rays</strong></td>
<td></td>
</tr>
<tr>
<td>photons</td>
<td>dipole</td>
</tr>
<tr>
<td></td>
<td>photoelectric absorption</td>
</tr>
<tr>
<td><strong>neutrons</strong></td>
<td>strong force</td>
</tr>
<tr>
<td></td>
<td>magnetic</td>
</tr>
<tr>
<td></td>
<td>neutron capture</td>
</tr>
<tr>
<td><strong>electrons</strong></td>
<td>Coulomb force</td>
</tr>
</tbody>
</table>
### Radiation – x-rays (photons), neutrons, electrons

<table>
<thead>
<tr>
<th></th>
<th>energy</th>
<th>wavelength</th>
<th>velocity</th>
<th>temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>x-rays</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>photons</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CuKa1</td>
<td>8.048 keV</td>
<td>1.54 A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MoKa1</td>
<td>17.479 keV</td>
<td>0.71 A</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>neutrons</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>thermal</td>
<td>25 meV</td>
<td>1.8 A</td>
<td>2200 m/s</td>
<td>293.6 K</td>
</tr>
<tr>
<td>cold</td>
<td>6.6 meV</td>
<td>3.5 A</td>
<td>1127 m/s</td>
<td>77 K</td>
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<tr>
<td><strong>electrons</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SEM</td>
<td>20 keV</td>
<td>0.122 A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TEM</td>
<td>200 keV</td>
<td>0.025 A</td>
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</tr>
</tbody>
</table>
Radiation – attenuation - Beer Lambert law

\[ I(x) = I_0 \exp(-\mu x) \]

Calculated for X-Rays \( E = 17500\text{eV} \)
Radiation – attenuation - Beer Lambert law

Scattering (elastic, inelastic) Absorption

\[ I(x) = I_0 \exp(-\mu x) \]

\[ \mu = \mu_a + \mu_s \]
Attenuation X-Rays: microscopic view

- **Photoelectric absorption**

- **Elastic (Rayleigh) Scattering**

- **Inelastic (Compton) Scattering**
X-Rays cross section magnitude

\[ I(x) = I_0 \exp(-\mu x) \]

\[ \mu = \sigma_c + \sigma_i + \tau \]

Data from:
H. Ebel, R. Svagera, M. F. Ebel, A. Shaltout and J. H. Hubbell,
Numerical description of photoelectric absorption coefficients for fundamental parameter programs,
X-Rays

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Atomic binding energies, electron energy levels

Absorption edges
Electron energy levels
Shells

<table>
<thead>
<tr>
<th>shell</th>
<th>n</th>
<th>l</th>
<th>j</th>
<th>spin sign</th>
<th>max number of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>1</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>L1</td>
<td>2</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>L2</td>
<td>2</td>
<td>1</td>
<td>0.5</td>
<td>-1</td>
<td>2</td>
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<tr>
<td>L3</td>
<td>2</td>
<td>1</td>
<td>1.5</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>M1</td>
<td>3</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>M2</td>
<td>3</td>
<td>1</td>
<td>0.5</td>
<td>-1</td>
<td>2</td>
</tr>
<tr>
<td>M3</td>
<td>3</td>
<td>1</td>
<td>1.5</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>M4</td>
<td>3</td>
<td>2</td>
<td>1.5</td>
<td>-1</td>
<td>4</td>
</tr>
<tr>
<td>M5</td>
<td>3</td>
<td>2</td>
<td>2.5</td>
<td>1</td>
<td>6</td>
</tr>
</tbody>
</table>

Z shell  energy_eV  jump  level_width_eV
79 K  80724.9  4.874  52.1
79 L1 14352.8  1.15567 9.8
79 L2 13733.6  1.4  5.53
79 L3 11918.7  2.55  5.54
79 M1 3424.9  1.04  15.0
79 M2 3147.8  1.058  9.5
79 M3 2743.0  1.15776 8.5
79 M4 2291.1  1.07  2.18
79 M5 2205.7  1.092  2.18

www.txrf.org/xraydata
Secondary effects – fluorescence vs Auger

Data from:
M. O. Krause,
X-Ray Fluorescence – characteristic lines

Siegbahn = Manne Siegbahn (swedish physicist)  
Nobel Prize in Physics in 1924

IUPAC = International Union of Pure and Applied Chemistry

<table>
<thead>
<tr>
<th>Siegbahn</th>
<th>IUPAC</th>
<th>Siegbahn</th>
<th>IUPAC</th>
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<tbody>
<tr>
<td>Kα₁</td>
<td>K-L3</td>
<td>Lα₁</td>
<td>L3-M5</td>
</tr>
<tr>
<td>Kα₂</td>
<td>K-L2</td>
<td>Lα₂</td>
<td>L3-M4</td>
</tr>
<tr>
<td>Kβ₁</td>
<td>K-M3</td>
<td>Lβ₁</td>
<td>L2-M4</td>
</tr>
<tr>
<td>Kβ₂</td>
<td>K-N2,N3</td>
<td>Lβ₂</td>
<td>L3-N5</td>
</tr>
<tr>
<td>Kβ₃</td>
<td>K-M2</td>
<td>Lβ₃</td>
<td>L1-M3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Lβ₄</td>
<td>L1-M2</td>
</tr>
</tbody>
</table>

Germanium

<table>
<thead>
<tr>
<th>Line</th>
<th>Energy [keV]</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kα₁</td>
<td>9.887</td>
<td>0.57380</td>
</tr>
<tr>
<td>Kα₂</td>
<td>9.856</td>
<td>0.29550</td>
</tr>
<tr>
<td>Kβ₁</td>
<td>10.983</td>
<td>0.08470</td>
</tr>
<tr>
<td>Kβ₂</td>
<td>11.103</td>
<td>0.00280</td>
</tr>
<tr>
<td>Kβ₃</td>
<td>10.978</td>
<td>0.04320</td>
</tr>
</tbody>
</table>
X-Ray Fluorescence – intensity - Sherman equation

\[ dI_{\zeta jk} \propto e^{-\mu_s, E_0 \frac{z}{\sin \phi_i}} W_{\zeta} \left( \frac{\tau_j}{\rho} \right) \zeta_{\bar{E}_0} \rho_s dz \]

- 1. attenuation to depth \( z \)
- 2. photoelectric absorption in layer \( dz \)
- 3. fluorescence yield
- 4. transition probability (relative intensity of lines in shell)
- 5. attenuation to the detector
- 6. detector efficiency

\[ I_0 G_0 G_1 \]

geometrical factors and primary flux form the element independent proportionality constant.
Modelling the response function of energy dispersive X-ray spectrometers with silicon detectors
F. Scholze, and M. Procop
Electrons interaction with matter


http://serc.carleton.edu/research_education/geochemsheet/s/electroninteractions.html
Inner shell ionization cross section: x-rays vs electrons

Cu K-shell photoelectric cross section

Cross Section (Barns)

energy / keV

atomic photoabsorption cross section / barn

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Volume 107, Number 6, November–December 2002
Journal of Research of the National Institute of Standards and Technology
Fig. 12.2 Various categories of neutron interactions. The letters separated by commas in the parentheses show the incoming and outgoing particles.
Cross section: x-rays vs neutrons

https://www.psi.ch/niag/comparison-to-x-ray
### Cross section: x-rays vs neutrons

#### Attenuation coefficients for thermal neutrons [cm⁻¹]

<table>
<thead>
<tr>
<th>1a</th>
<th>2a</th>
<th>3b</th>
<th>4b</th>
<th>5b</th>
<th>6b</th>
<th>7b</th>
<th>8</th>
<th>1b</th>
<th>2b</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>3.44</td>
<td>Li</td>
<td>3.30</td>
<td>Be</td>
<td>0.79</td>
<td>0.15</td>
<td>0.09</td>
<td>0.15</td>
<td>0.09</td>
</tr>
<tr>
<td>K</td>
<td>0.06</td>
<td>Ca</td>
<td>0.08</td>
<td>Sc</td>
<td>2.00</td>
<td>0.60</td>
<td>0.72</td>
<td>0.54</td>
<td>1.21</td>
</tr>
<tr>
<td>Rb</td>
<td>0.08</td>
<td>Sr</td>
<td>0.14</td>
<td>Y</td>
<td>0.27</td>
<td>0.29</td>
<td>0.40</td>
<td>0.52</td>
<td>0.17</td>
</tr>
<tr>
<td>Cs</td>
<td>0.29</td>
<td>Ba</td>
<td>0.07</td>
<td>La</td>
<td>0.55</td>
<td>4.99</td>
<td>1.49</td>
<td>1.47</td>
<td>6.85</td>
</tr>
<tr>
<td>Fr</td>
<td>0.34</td>
<td>Ra</td>
<td>Ac</td>
<td>0.14</td>
<td>0.41</td>
<td>1.87</td>
<td>6.72</td>
<td>171.47</td>
<td>94.58</td>
</tr>
</tbody>
</table>

#### Attenuation coefficients for X-ray [cm⁻¹] (150kV)

<table>
<thead>
<tr>
<th>1a</th>
<th>2a</th>
<th>3b</th>
<th>4b</th>
<th>5b</th>
<th>6b</th>
<th>7b</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.02</td>
<td>Li</td>
<td>0.06</td>
<td>Be</td>
<td>0.22</td>
<td>0.13</td>
<td>0.24</td>
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<tr>
<td>K</td>
<td>0.14</td>
<td>Ca</td>
<td>0.26</td>
<td>Sc</td>
<td>0.48</td>
<td>0.73</td>
<td>1.04</td>
</tr>
<tr>
<td>Rb</td>
<td>0.47</td>
<td>Sr</td>
<td>0.86</td>
<td>Y</td>
<td>1.61</td>
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<td>3.43</td>
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<tr>
<td>Cs</td>
<td>1.42</td>
<td>Ba</td>
<td>2.73</td>
<td>La</td>
<td>5.04</td>
<td>9.70</td>
<td>25.47</td>
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<tr>
<td>Fr</td>
<td>11.80</td>
<td>Ra</td>
<td>Ac</td>
<td>24.47</td>
<td>Rf</td>
<td>Ha</td>
<td></td>
</tr>
</tbody>
</table>

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https://www.psi.ch/niag/comparison-to-x-ray
Scattering (full line) and absorption (dotted) cross sections of light element commonly used as neutron moderators, reflectors and absorbers, the data was obtained from database NEA NENDF/B-VII.1 using JANIS software.

https://en.wikipedia.org/wiki/Neutron_cross_section
Scattering - Differential cross section

\[
\frac{d\sigma}{d\Omega}
\]

incident beam with macroscopic width

case sample

d\Omega = d\theta d\phi

http://www.physics.csbsju.edu/QM/square.17.html
X-Rays - Differential cross section – elastic scattering

elastic scattering at MoKa1

elastic scattering at CuKa1

θ angle / deg

θ angle / deg
X-Rays - Differential cross section – inelastic scattering

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Electrons - Differential elastic cross section

Data from: http://www.ioffe.rssi.ru/ES/Elastic/
X-ray differential elastic cross section and the form factor

\[ \frac{d\sigma_{el}}{d\Omega} = \frac{d\sigma_T}{d\Omega} |F(x, Z)|^2 \]

Thomson cross section

\[ \frac{d\sigma_T}{d\Omega} = \frac{r_0^2}{2} (1 + \cos^2 \theta) \]

Atomic form factor (atomic scattering factor)

Variable related to the momentum transfer

\[ F(x, Z) \quad x = \frac{\sin \frac{\theta}{2}}{\lambda} \quad F(x, Z) = 4\pi \int_0^\infty r^2 \rho(r, Z) \frac{\sin(4\pi x r)}{4\pi x r} dr \]
X-ray differential elastic cross section and the form factor

... but actually there is a further dependence on energy ...

\[ f = f^0(x, Z) + f'(E, Z) + if''(E, Z) \]

\( f'' \)  photoelectric absorption
\( f' \)  corrections for photoabsorption (Kramers-Kronig dispersion)
relativistic effects, nuclear scattering

Diffraction (structure factor)

\[ F(h, k, l) = \sum_j f_j e^{-M_j} e^{2\pi i(hx_j + ky_j + lz_j)} \]
forward scattering factors \((x = \theta = q = 0)\)

\[
f = f(0, Z, E) = f_1 + if_2
\]

\[
f_2 \equiv f''
\]

\[
f_1 \equiv f^0(x = 0) + f'
\]

\[
\mu_a = 2r_0 \lambda f_2
\]

F1 and F2 are directly related to the index of refraction (reflection, refraction, XRR)

\[
n = 1 - \frac{1}{2\pi} Nr_0 \lambda^2 (f_1 + if_2)
\]

\[
n = 1 - \delta - i\beta
\]
X-ray differential inelastic cross section (Compton)

\[
\frac{d\sigma_i}{d\Omega} = \frac{d\sigma_{KN}}{d\Omega} S(q, Z)
\]

\[
\frac{d\sigma_{KN}}{d\Omega} = \frac{r_0^2}{2} P(\theta, E)
\]

\[
P(\theta, E) = \frac{1}{(1 + \alpha(1 - \cos \theta))^2} \left[ 1 + \cos^2 \theta + \frac{\alpha^2(1 - \cos \theta)^2}{1 + \alpha(1 - \cos \theta)} \right]
\]

\[
\alpha = \frac{E}{m_0 c^2}
\]

\[
S(q, Z) = \int_{\varepsilon > 0} \left| F_\varepsilon (q, Z) \right|^2
\]

Inelastic scattering function

\[
F_\varepsilon (\vec{q}, Z) = \sum_{n=1}^{Z} \langle \Psi_\varepsilon | \exp(i\vec{q} \cdot \vec{r}_n) | \Psi_0 \rangle
\]

Form factor elastic scattering

\[
F(\vec{q}, Z) = \sum_{n=1}^{Z} \langle \Psi_0 | \exp(i\vec{q} \cdot \vec{r}_n) | \Psi_0 \rangle
\]
In a spectrum the Compton peak is broader due to the angle dependence (in the accepted solid angle there are different scattering angles) and due to Doppler broadening.
X-Ray Absorption near edge fine structure

The X-ray Absorption Fine Structure (XAFS) of an iron foil

Different phenomena for:
- ‘free’ atoms
- molecules
- condensed systems
X-Ray Absorption near edge fine structure

\[ E_{ph} \sim E_b \]

Core electron
unoccupied levels

⇒ Edge fine structure
(XANES or NEXAFS)

\[ E_{ph} > E_b \]

Core electron
continuum
outgoing wavefunction

Extended fine structure
(EXAFS)

INTERFERENCE
incoming wavefunction

Backscattering
from neighbouring atoms

\[ \mu (\text{a.u.}) \]

Photon energy (keV)

Ge
Thank you for your attention!