X-ray production in the TEM

Lecture 18

What is an x-ray?

X-rays are electromagnetic radiation

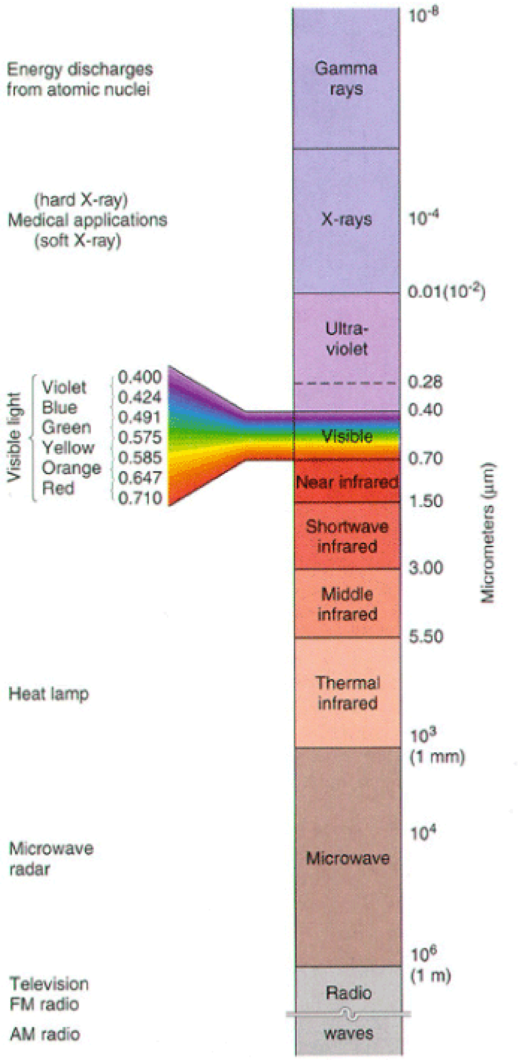
- Can be considered as either photons or waves

Wavelengths between 100 nm (“soft”) and 100 pm (“hard”)

Like all photons:

$$\lambda = \frac{hc}{eE}$$

λ = wavelength
h = Planck’s constant
c = speed of light
e = electron charge
E = energy



source: Christopherson (2000) *Geosystems*

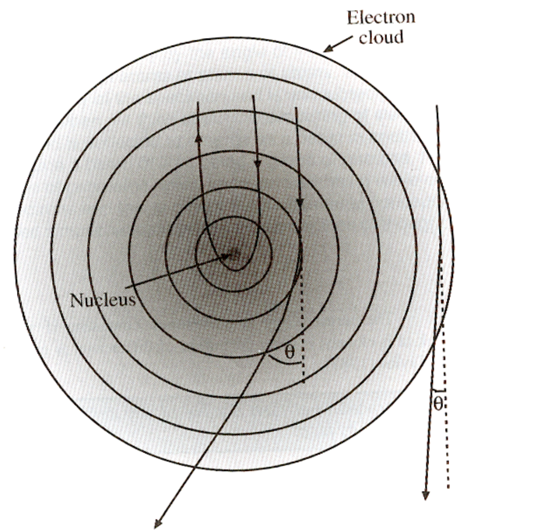
Bremsstrahlung X-ray emission

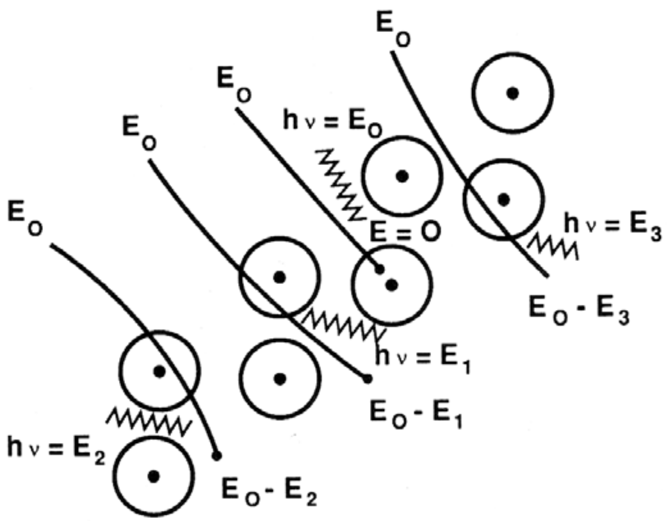
"Braking" radiation

Electron is decelerated by Coulomb (charge) field of the nucleus

Electromagnetic radiation (x-ray) is emitted

Can have any energy less than the incident energy

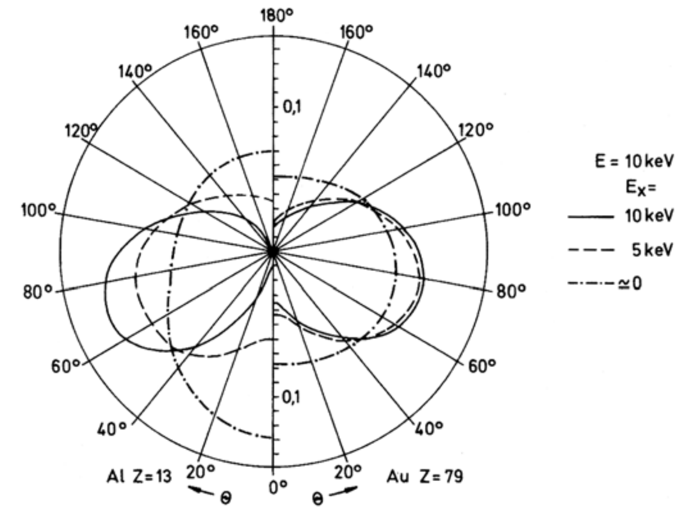


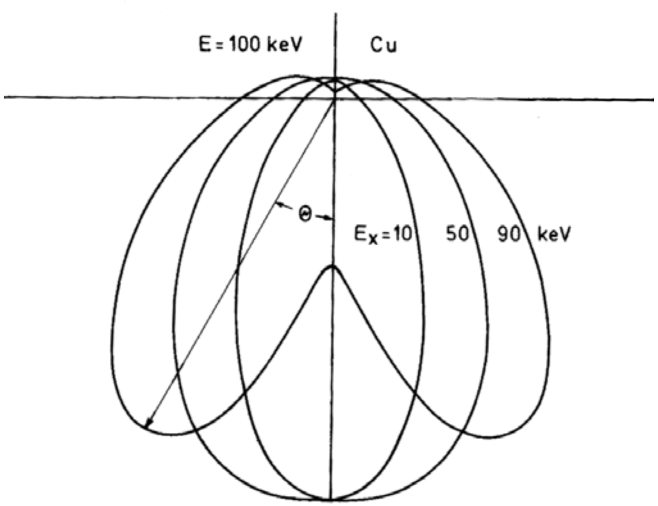


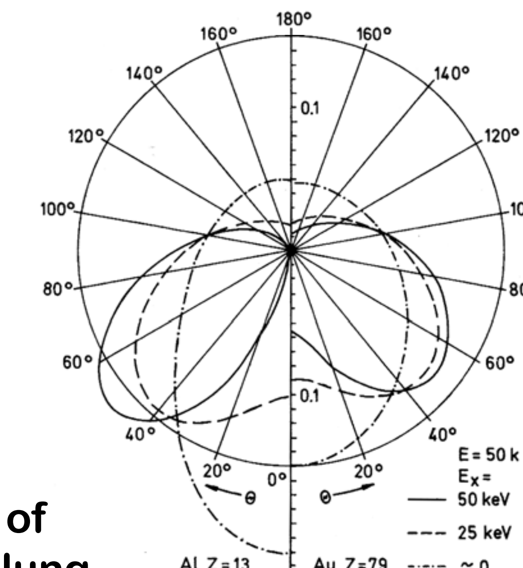
Bremsstrahlung X-ray emission

Resulting x-ray emission is forward peaked

– As incident electron energy goes, up the x-ray emission is more strongly forward peaked.





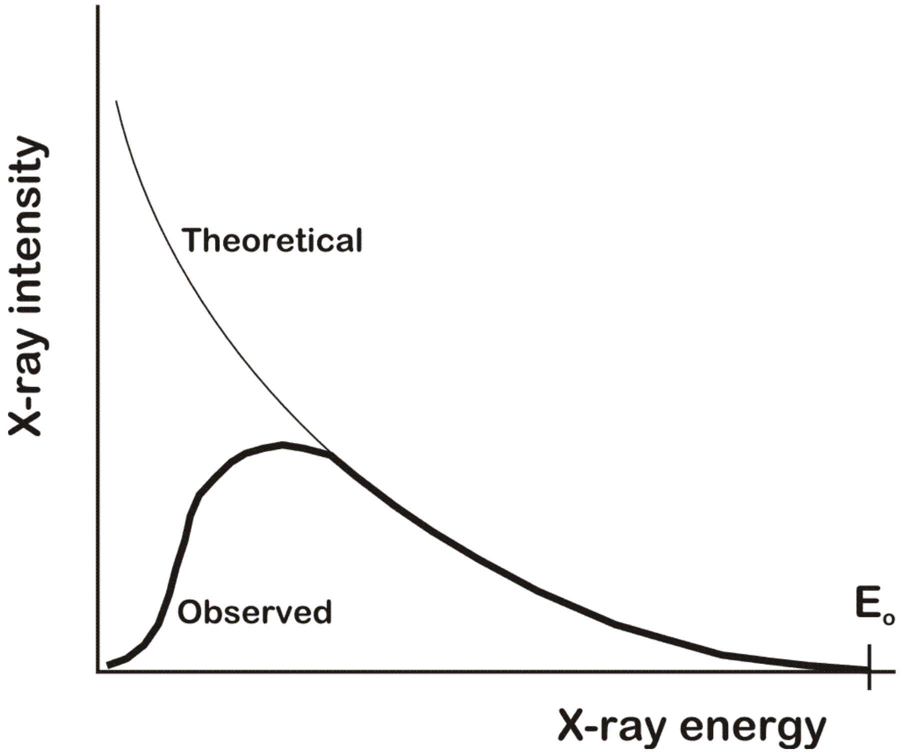


Angular distribution of Bremsstrahlung scatter

Bremsstrahlung X-ray emission

Results in a continuous background signal in an intensity vs. energy spectrum

Extends from low energies to up to the incident beam energy



Bremsstrahlung X-ray emission

Why do we care?

1. **Forms a background signal under the signal of interest**
   - Once a photon is created with a given energy, we cannot know what caused it
     - In other words, did the count in our spectrometer at a given energy come from a bremsstrahlung x-ray or a characteristic x-ray
   - Generally, this is nuisance in x-ray spectroscopy
2. **But, carries information about the atomic number of the specimen**
   - Can be useful in biological analyses

Reminder: quantum numbers

Atom composed of positively charged nucleus, surrounded by electrons

Each electrons has a given energy

- Described by quantum numbers
- These are the eigen-solutions to the Schrödinger Equation:

$$n = 1,2,3....$$

$$\mathrm{l} = 0,1,2, ..., n\text{-}1$$

$$j = \mathrm{l} + s, \quad \text{where } s = \pm \tfrac{1}{2}$$

$$m_j \leq |j|$$

Electrons subject to Pauli's Exclusion Principle:

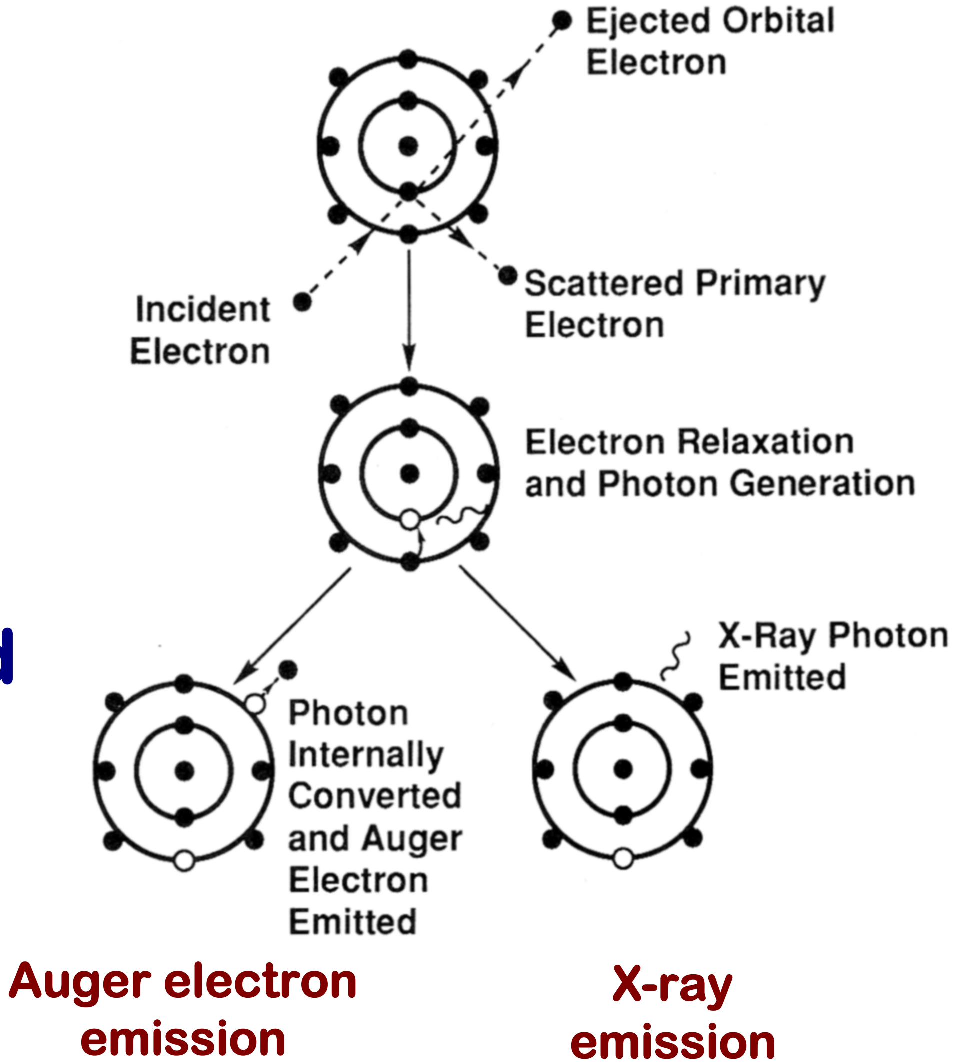
- No two electrons can have the exact same set of quantum numbers (and thus same energy)

Inner shell ionization

Incident electron imparts sufficient energy to an electron in an atom to remove if from it's "shell"

Atom is left in an excited state

Atom relaxes to ground state through a limited set of transitions

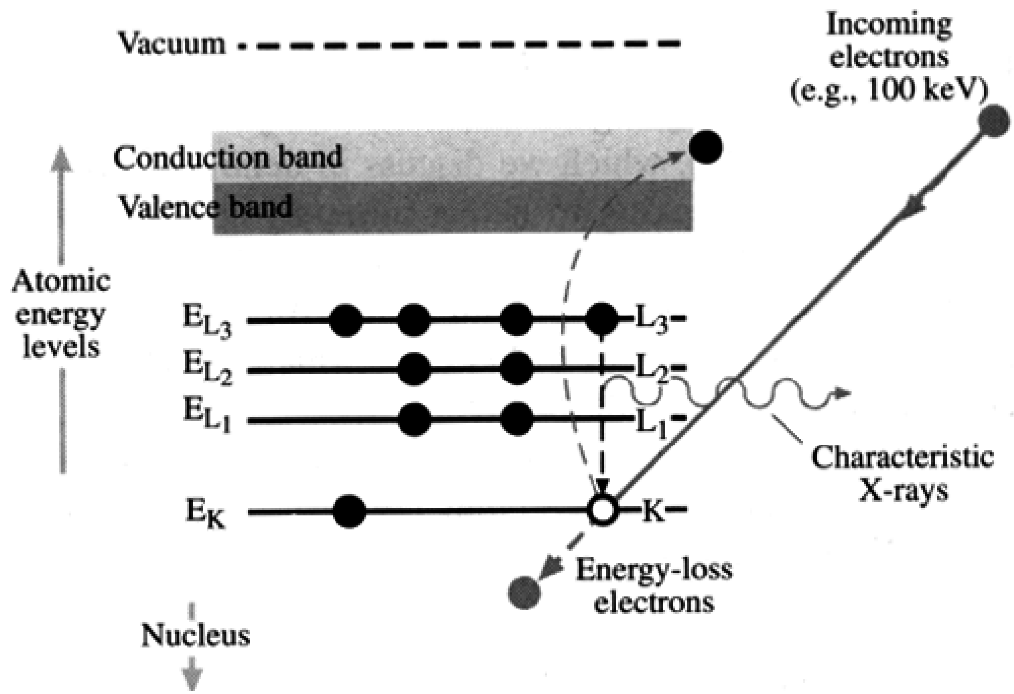


http://www.matter.org.uk/tem/electron_atom_interaction/x-ray_and_auger.htm

Characteristic X-rays

One such transition is:

1. Incident electron ionizes atom
2. Electron from outer shell fills the hole left in the inner shell
3. Results in the emission of an x-ray



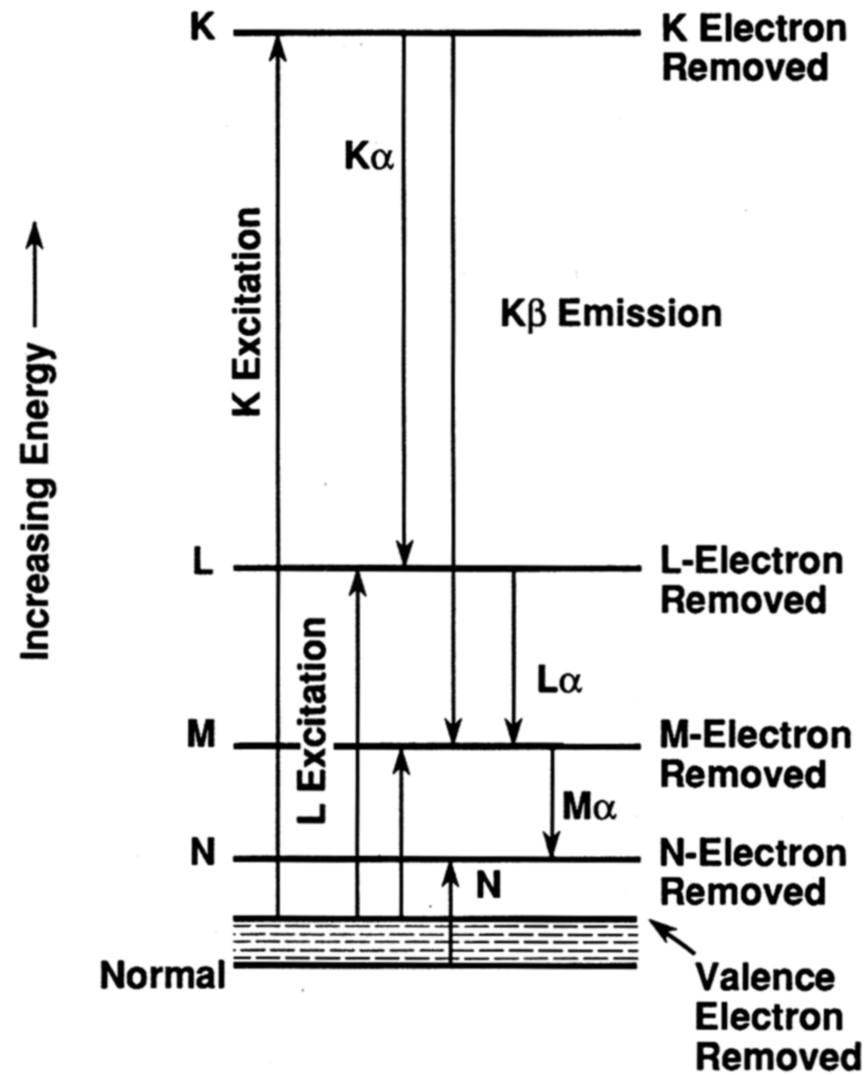
<u>Importantly</u>, the energy of the resultant x-ray is *characteristic* of the atom

- Energy levels are specific to each atom
- Thus difference between energy levels is also

Characteristic X-rays

Nomenclature used is ‘spectroscopic’

- K shell ⇧ $n = 1$
- L shell ⇧ $n = 2$
- M shell ⇧ $n = 3$
- N shell ⇧ $n = 4$



Reminder: spectroscopic notation

Shells and Subshells of Atoms

X-ray notation	Quantum numbers				Maximum electron population
	n	l	j	m_j	
K	1	0	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
L_{I}	2	0	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
L_{II}	2	1	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
L_{III}	2	1	$\frac{1}{2}$	$\pm\frac{3}{2}, \pm\frac{1}{2}$	4
M_{I}	3	0	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
M_{II}	3	1	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
M_{III}	3	1	$\frac{3}{2}$	$\pm\frac{3}{2}, \pm\frac{1}{2}$	4
M_{IV}	3	2	$\frac{3}{2}$	$\pm\frac{3}{2}, \pm\frac{1}{2}$	4
M_{V}	3	2	$\frac{5}{2}$	$\pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$	6
N_{I}	4	0	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
N_{II}	4	1	$\frac{1}{2}$	$\pm\frac{1}{2}$	2
N_{III}	4	1	$\frac{3}{2}$	$\pm\frac{3}{2}, \pm\frac{1}{2}$	4
N_{IV}	4	2	$\frac{3}{2}$	$\pm\frac{3}{2}, \pm\frac{1}{2}$	4
N_{V}	4	2	$\frac{5}{2}$	$\pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$	6
N_{VI}	4	3	$\frac{5}{2}$	$\pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$	6
N_{VII}	4	3	$\frac{7}{2}$	$\pm\frac{7}{2}, \pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$	8

Characteristic X-rays

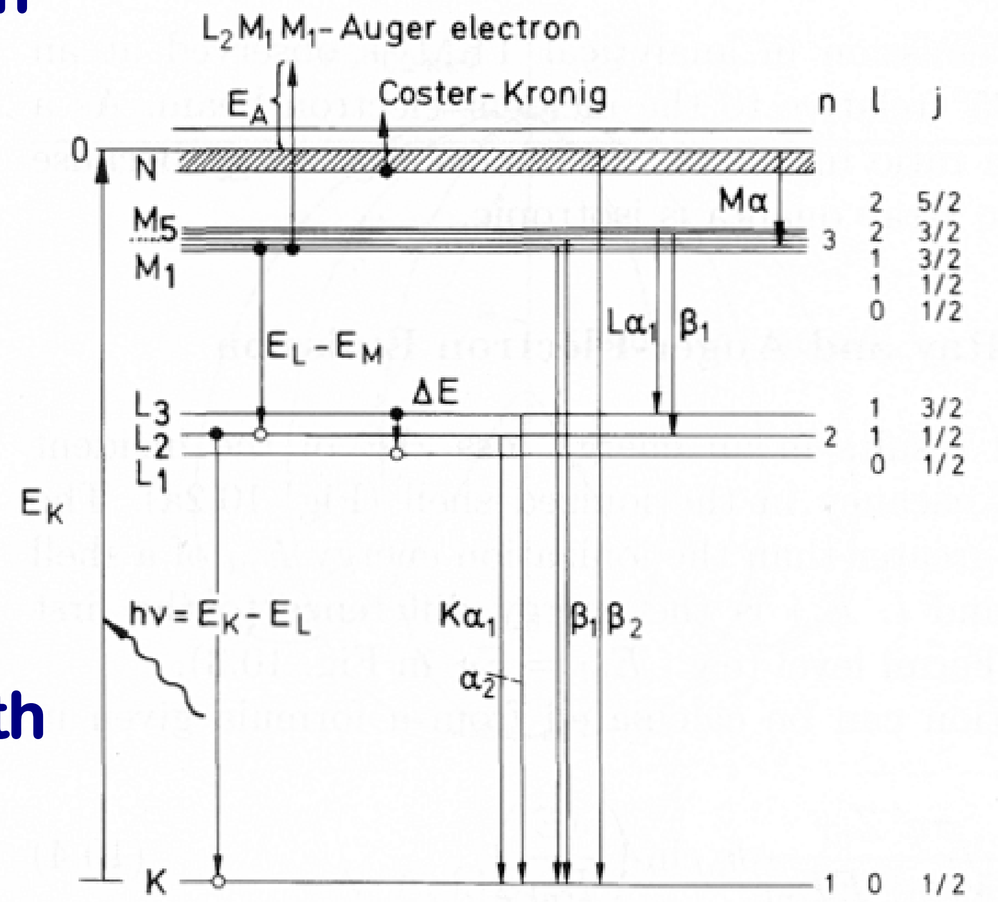
X-rays, as EM radiation can be considered as either waves or photons

Energy related to wavelength:

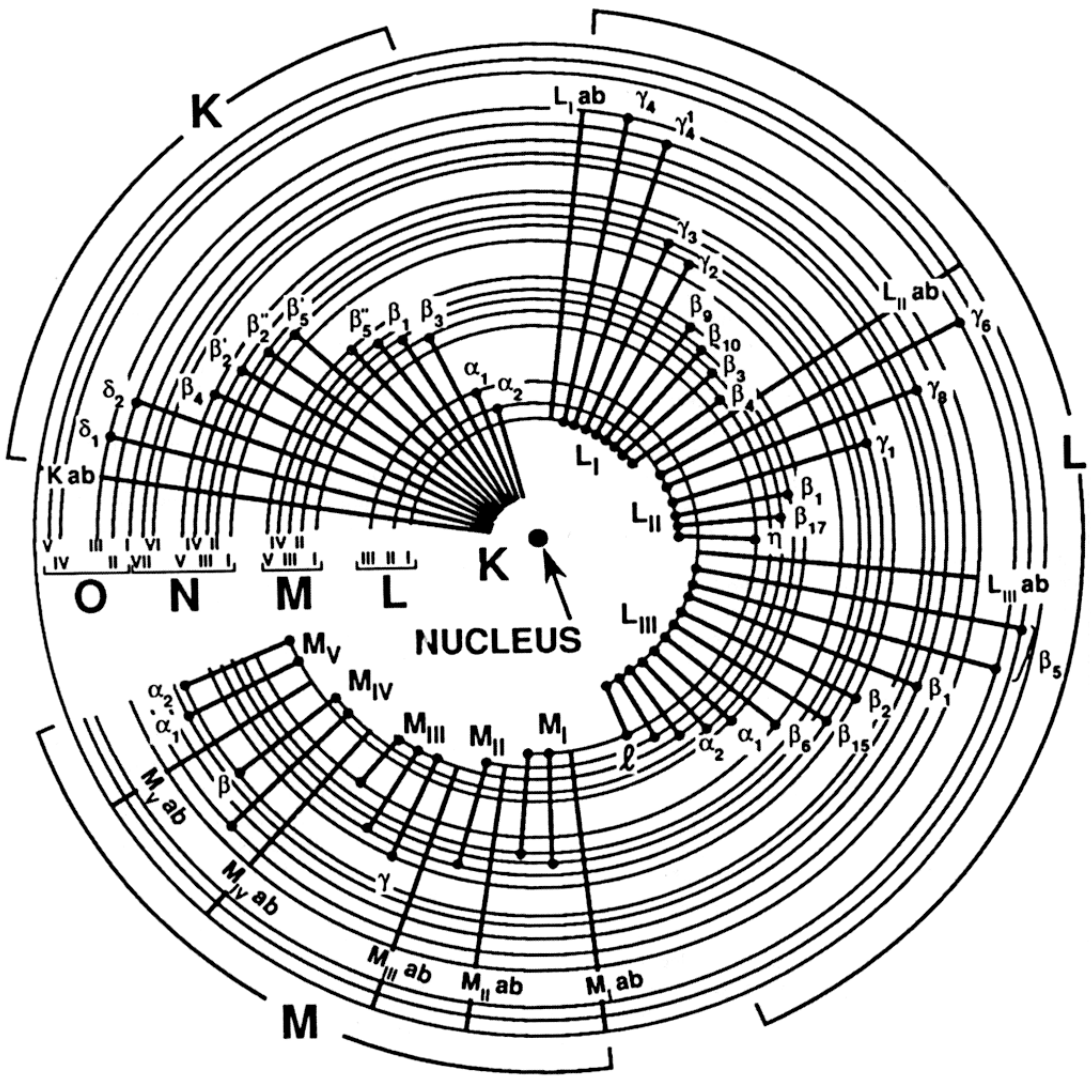
$$E = h\upsilon = \frac{hc}{\lambda}$$

Each transition has a specific energy & wavelength associated with it (E_K, E_L, E_M)

- $E_K, E_L, E_M < E_c$

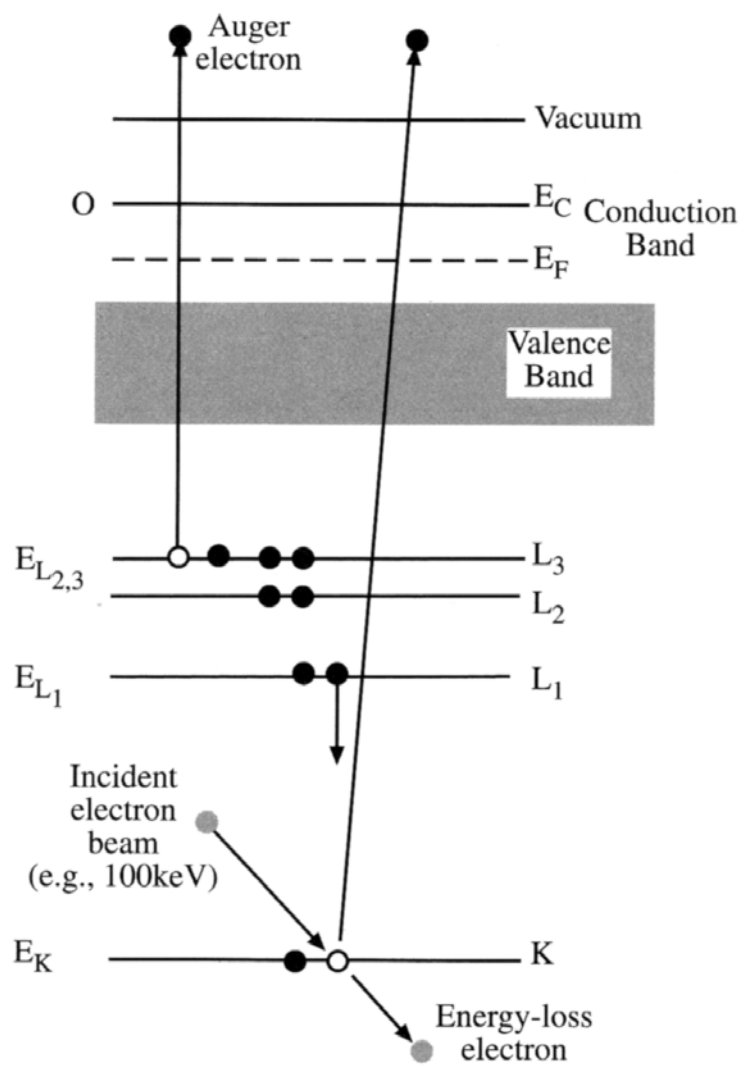


Characteristic X-rays

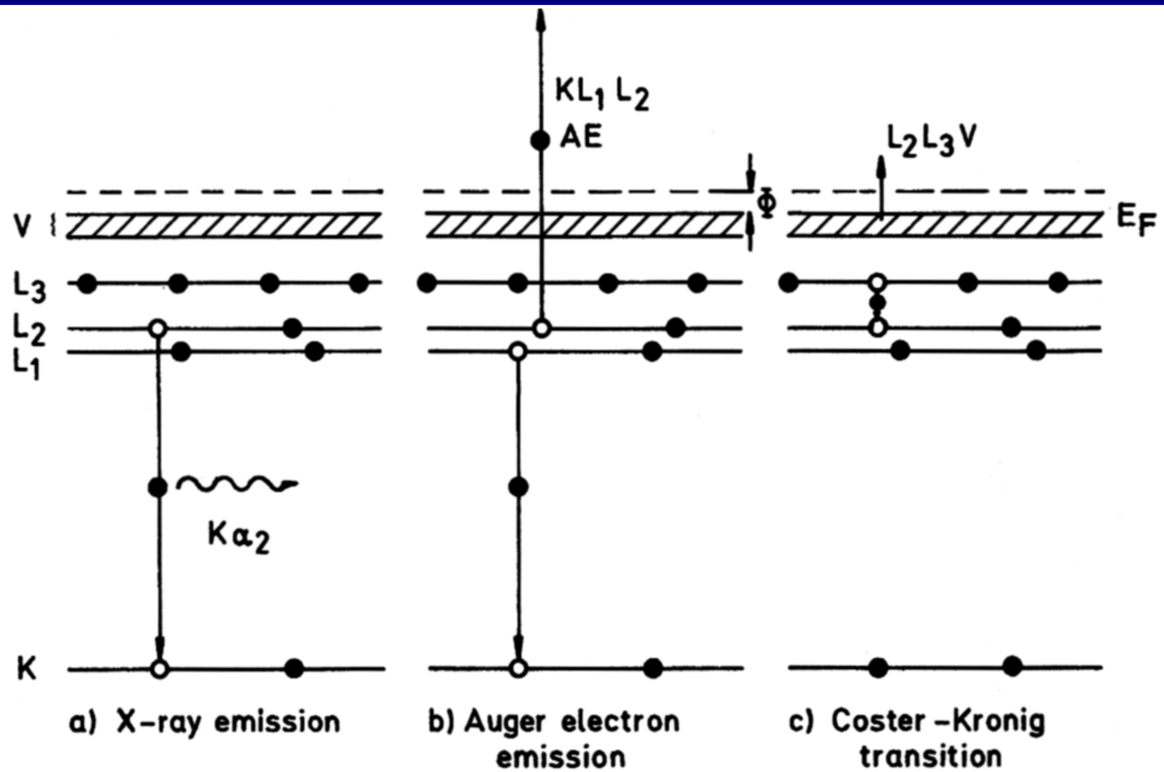


Auger electron emission

- Incident electron removes inner shell electron
- Outer shell electron fills empty hole
- Instead of x-ray emission, an electron from a higher shell is ejected
- These electrons have a characteristic energy
  - E_C-$E_{L2,3}$ in this case
  - Favored in light atoms
- Most Auger electrons are absorbed by the lattice
  - Only those at the surface escape
  - Auger spectroscopy (AES) requires UHV



Side note …



"Coster-Kronig" transition

- Transitions of electrons from a higher states in a sub-shell to vacancies in a lower sub-shell
- Energy transferred to an electron near the Fermi Level
- Can be important when considering fluorescence quantitatively (SEM)

Characteristic X-rays

Ionization requires a critical energy E_C

- K shell ionization energy > L shell > M shell …
- Varies with element (makes sense!)
- Note: ionization energy does not equal energy of the emitted x-ray

Critical Ionization Energies for Platinum

Shell	Critical ionization energy (keV)
K	78.39
L_I	13.88
L_{II}	13.27
L_{III}	11.56
M_I	3.296
M_{II}	3.026
M_{III}	2.645
M_{IV}	2.202
M_V	2.122

Can describe a cross-section (probability that ionization will occur)

- Mathematical form not of interest here
- Two useful outcomes
  - The electron that caused the ionization undergoes a small angular deviation
  - The resultant characteristic x-ray is emitted uniformly over 4π steradian

Fluorescence yield

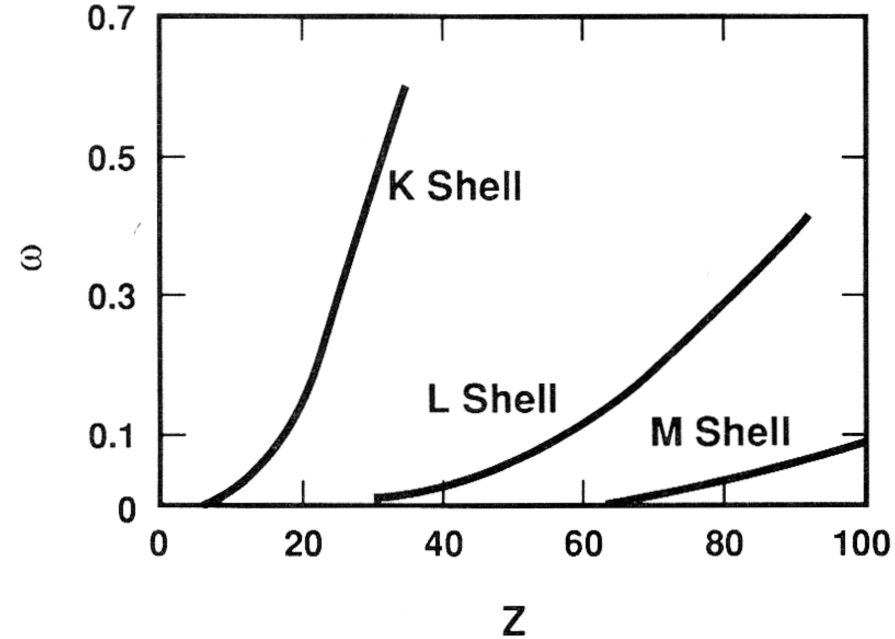
Partitioning between x-ray emission and Auger electron emission varies by element

Mathematically:

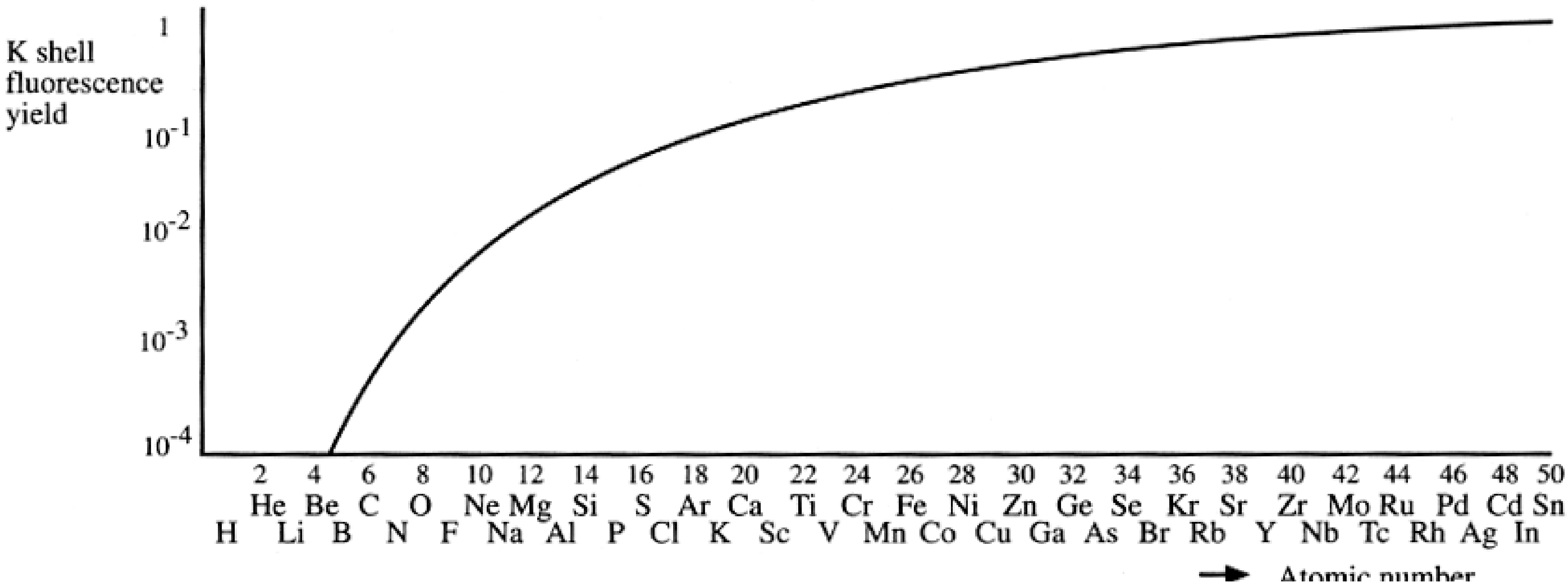
$$\omega + a = 1$$

Auger electron fluorescence yield

X-ray fluorescence yield



Fluorescence yield



Strong atomic # dependence:

– One C K_α X-ray generated per 1000 ionization events

– One Ge K_α X-ray generated per 2 ionization events

Fluorescence yield

Approximate probability of occurrence

K_α - 1	K_α - 0.1					
$L_{\alpha 1,2}$ - 1	$L_{\beta 1}$ - 0.1	$L_{\beta 1}$ - 0.2	$L_{\gamma 1}$ - 0.08	$L_{\gamma 3}$ - 0.03	L_α - 0.04	L_ν - 0.01
M_α - 1	M_β - 0.6	M_ξ -0.05	M_α - 0.08	$M_{II}N_{IV}$ - 0.01		

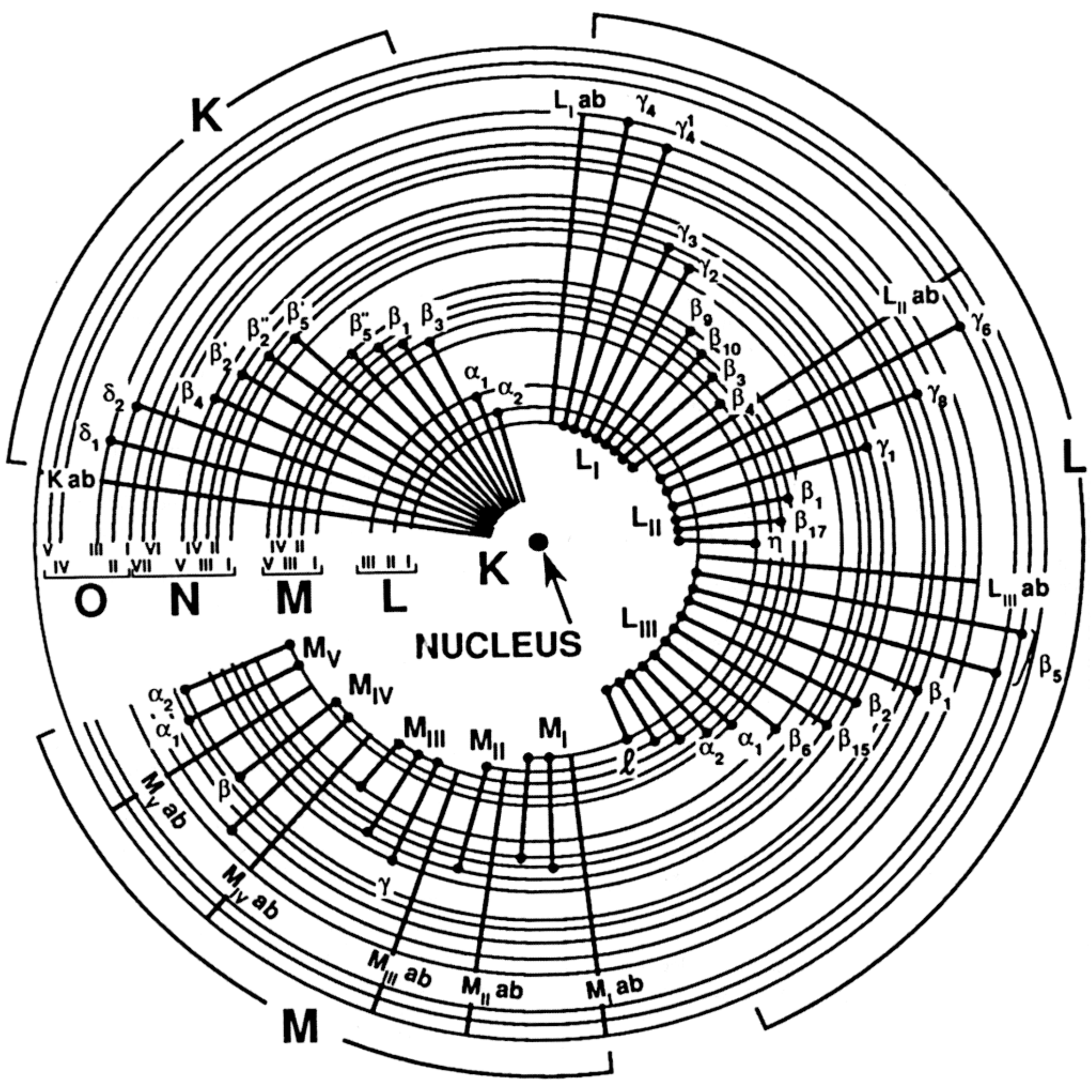
You are only likely to see the α & β lines of a given family

– Unless you have very good signal and take a long acquisition

Note, you cannot compare across families

– Relative probabilities between K, L, M & N vary with element

Characteristic X-rays



Characteristic X-ray Energy

Moseley's Law:

$$\lambda = \frac{B}{(Z - C)^2}$$

B&C are element specific constants