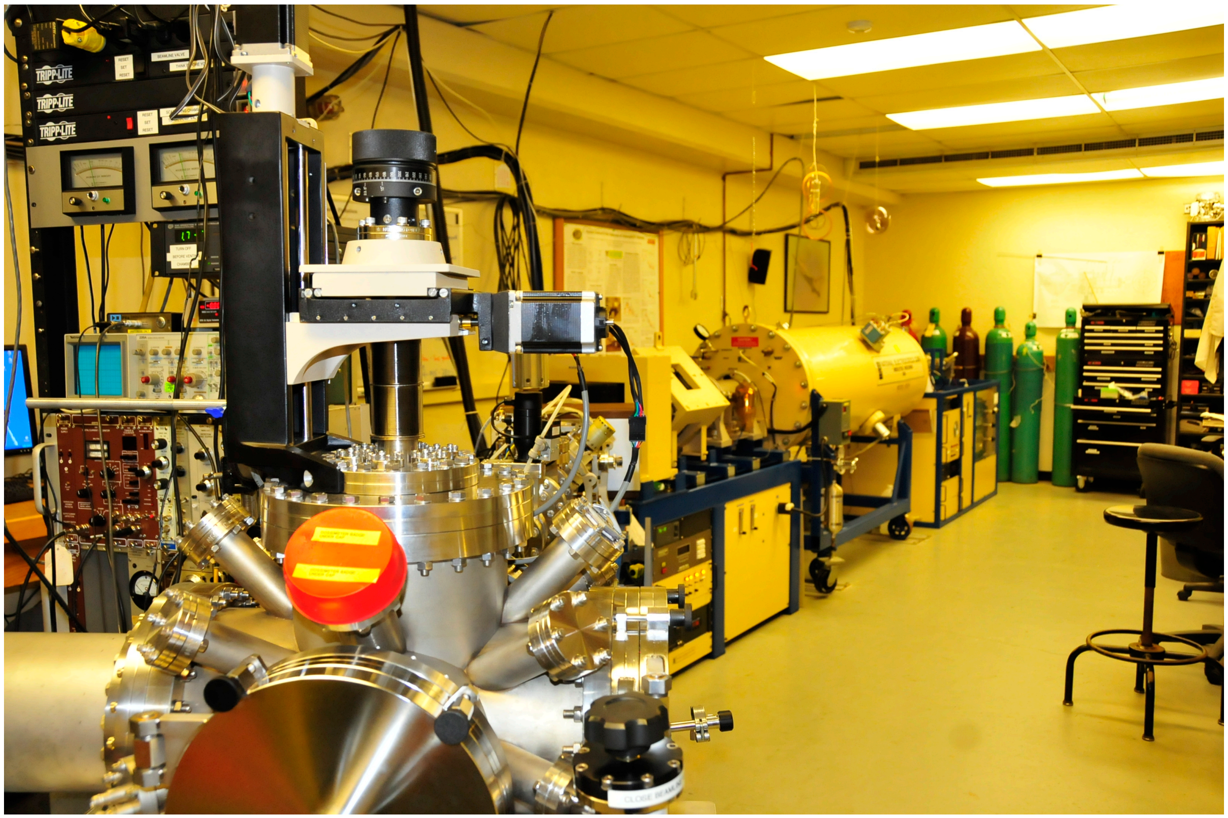
Materials Analysis with fast ions using the 1.1MV tandem electrostatic Pelletron Particle Accelerator at Union College



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Introduction to Ion Beam Analysis

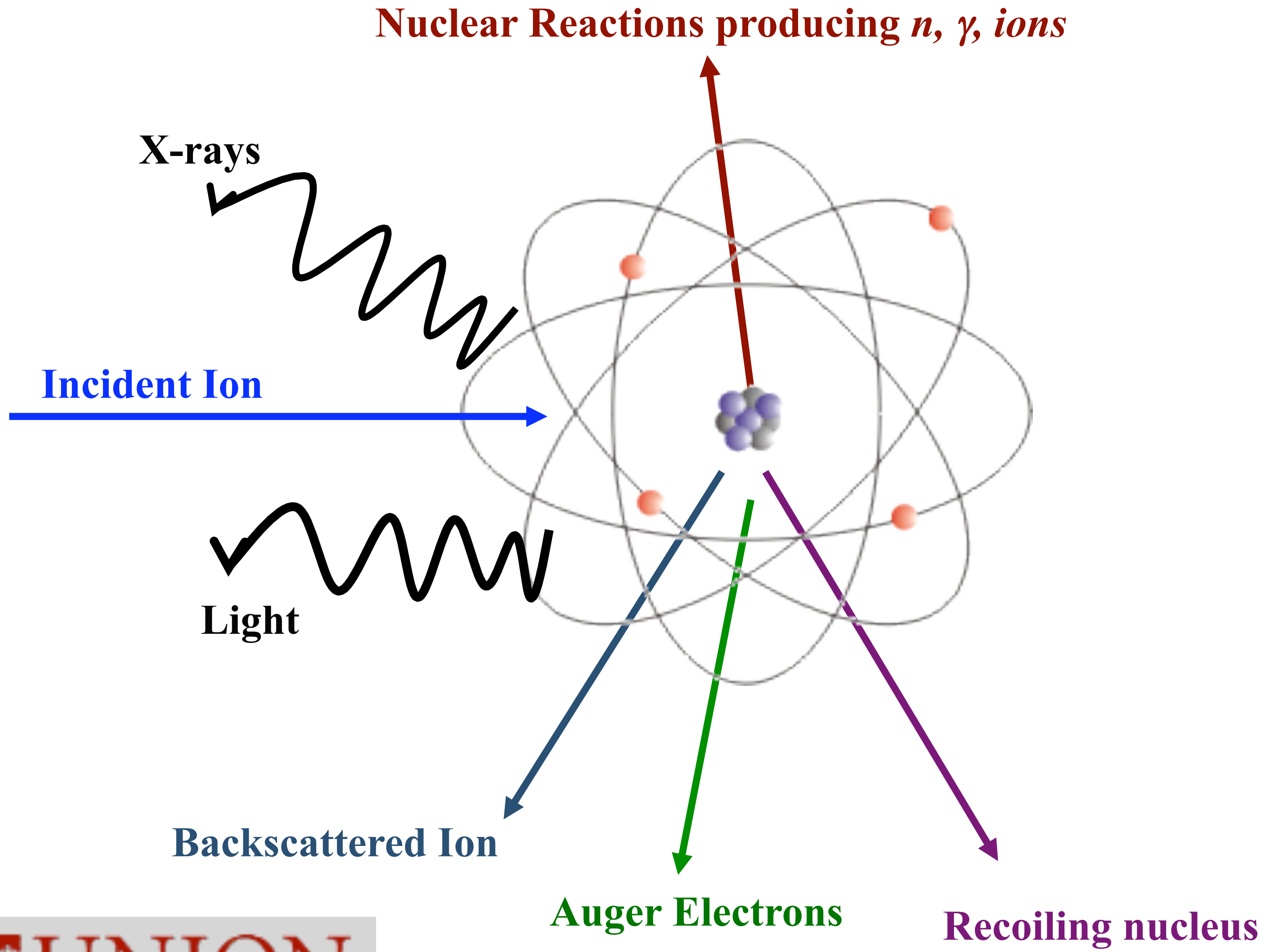
→ Ion –Target Interaction

- Elastic Atomic Collisions
  - Very low energies, typically a few *keV*
  - Surface composition and structure
  - Ion Scattering spectrometry (ISS)
- Inelastic Atomic Collisions
  - Ionization of target atoms
  - Characteristic x-ray emission
  - Particle Inducted X-Ray Emission (*PIXE*)
  - Detection of elements with $Z > 6$

- Elastic Nuclear Collisions
  - Rutherford Backscattering (*RBS*)
    - Mainly for $Z > Z_{ion}$ (usually He^{++})
  - Elastic Recoil Detection Analysis (*PESA*)
    - Mainly for $Z < Z_{ion}$ (only H in this case)
- Inelastic Nuclear Collisions
  - Nuclear Reactions can occur
    - Nuclear Reaction Analysis (NRA)
    - Gamma ray production (*PIGE*)

In our lab we have the ability to do *PIXE*, *PIGE*, *RBS* & PESA

Introduction: Ion –Target Interaction



Proton Induced X-ray Emission Spectroscopy

PIXE

- **First observation by Chadwick (the discover of the neutron)**
  (Phil. Mag. 24 (1912) 54)

- **X-ray emission induced by charged particles from a radioactive source.**
  - **We're going to produce protons on our accelerator and shoot them at a target to produce x rays.**

- **Moseley in1913: the energy of the x rays scales with Z^2**

- **First application T.B. Johansson et al, Nucl. Instr. Meth. B 84 (1970) 141**

- **2012: most widely used technique in materials analysis, atmospheric aerosols, archaeology, paleontology, archaeometry, criminology, biology, geology, environmental sciences.....**

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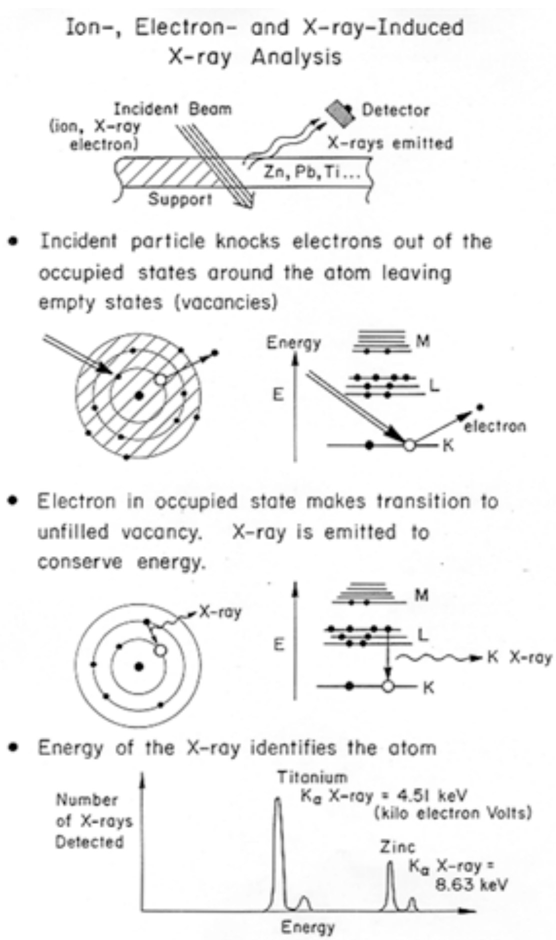
PIXE: The Basics



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Incident proton interacts with electrons in the material ejecting electrons.

This creates a vacancy in a shell that is usually filled with an electron from a higher orbit.

In order for the electron to fill this vacancy it needs to lose energy.

The energy difference is the difference from where the electron is currently to where it wants to go and this is typically on the order of several keV and higher.

When the electron transitions an x-ray photon of that energy difference is emitted and the spectrum of all x-ray photons are plotted and identified.

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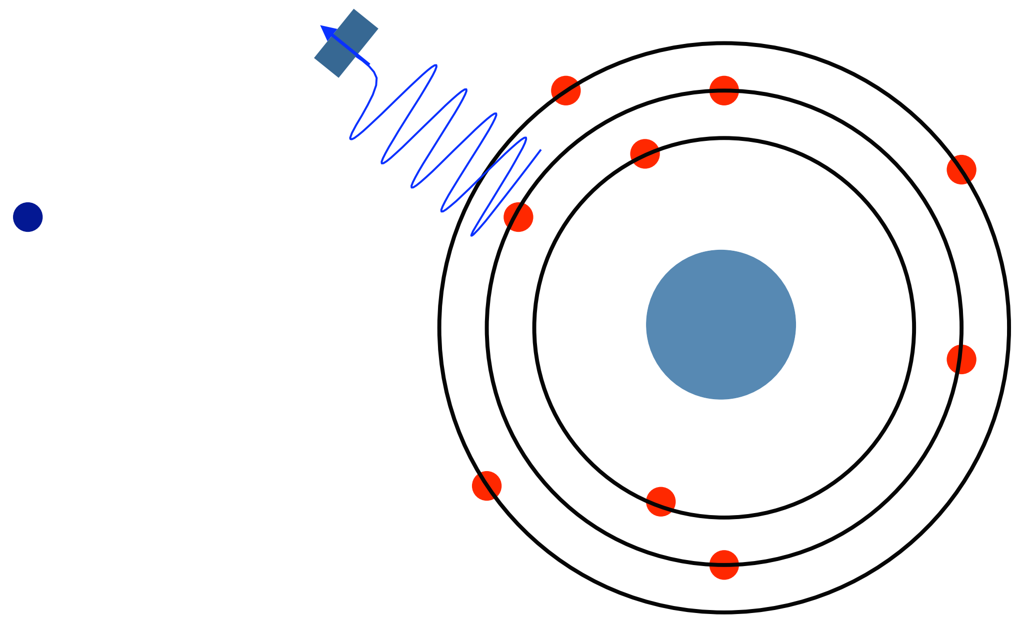
An Illustration of the *PIXE* process



L_α transition in an atom

PIXE: The Basics

- **For an incident proton energy of 1 – 4 MeV, elements with atomic numbers up to about 50 are generally determined through their *K shell* X-rays (typically K_α line).**

- **Heavier elements are measured through their *L shell* X rays because the energies of their *K shell* X rays are too high to be detected by using the Silicon detectors available commercially.**

- **The concentration of an element is deduced from the intensity of the measured X-ray line together with parameters obtained either theoretically and/or experimentally.**

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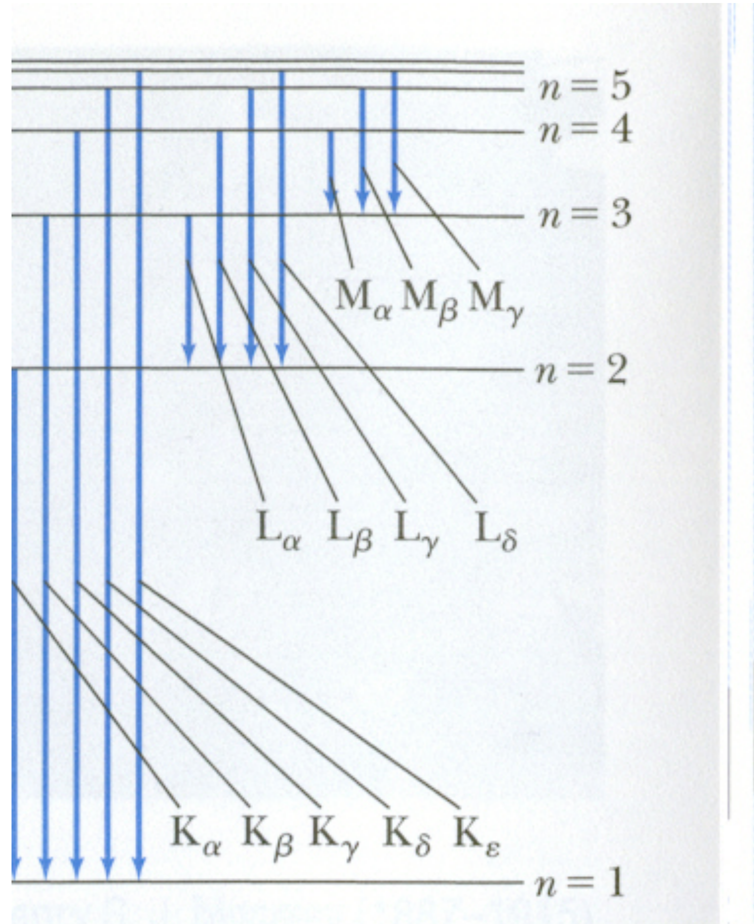
Characteristic X-ray production

Idea based on the *Bohr model of the atom*.

- **The energy of the photon emitted depends on the energy of the upper state and the energy of the lower state.**

$$\Delta E_{photon} = E_{upper} - E_{lower}$$

- **The *n* designations correspond to atomic orbitals while the letter designations (*K, L, M*…) correspond to shells in the older spectroscopic notation.**



Thornton, S., & Rex, A., Modern Physics for Scientists and Engineers, 3rd Ed., Thomas Brooks Cole 151(2006).

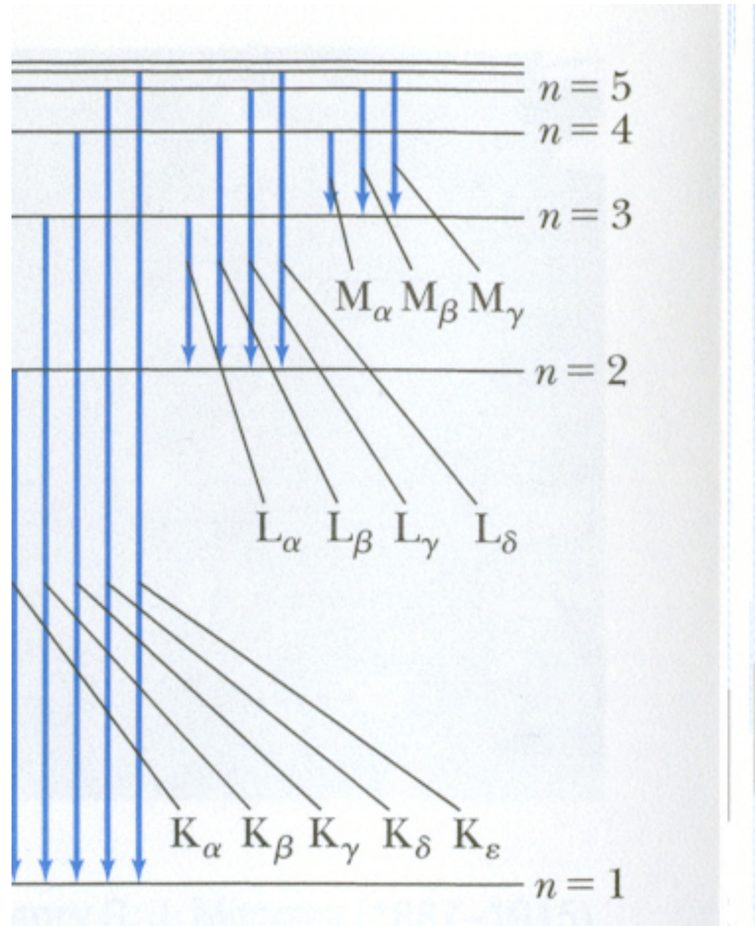
Characteristic X-ray production

• Further, the letters are used to designate the shell to which the electron is transitioning.

• The Greek letters are used to designate the higher energy transitions and give the value of Δn.

• For example, the α-transition is a lower energy (higher probability) transition than the β-transition (lower probability), which is in turn lower than the γ-transition.

• The K shell transitions are the highest energy transitions possible.



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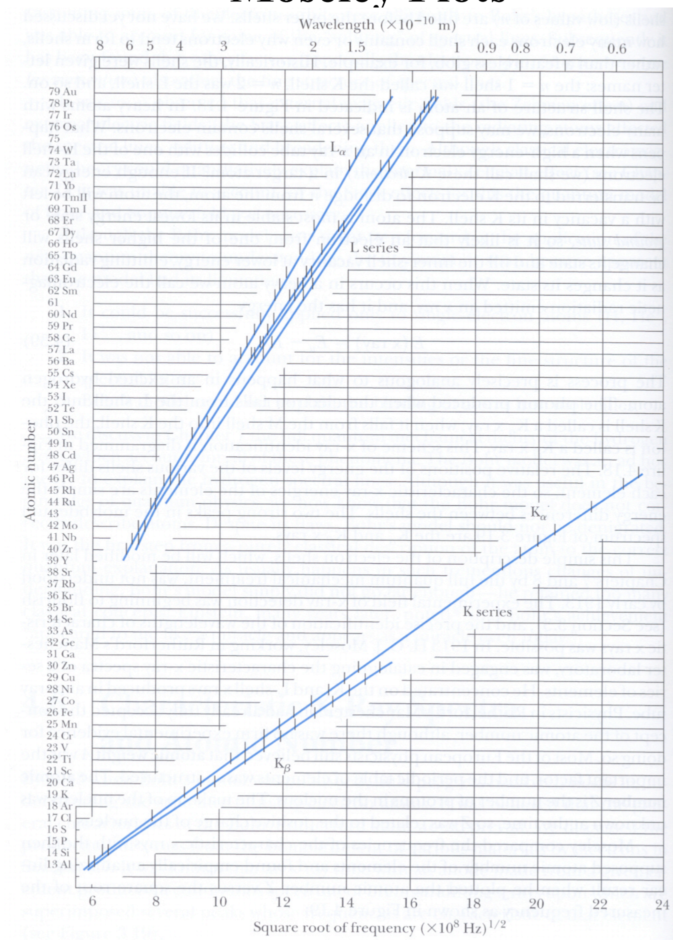
Characteristic X-ray production

- Moseley in 1913 empirically determined the relationship between the wavelength of the emitted x-ray and the atomic number. Plots like those on the right are called Moseley Plots

- This is the most fundamental idea behind PIXE.

- It shows that for each atomic number (element) there are a characteristic set of x-ray wavelengths emitted.

Moseley Plots



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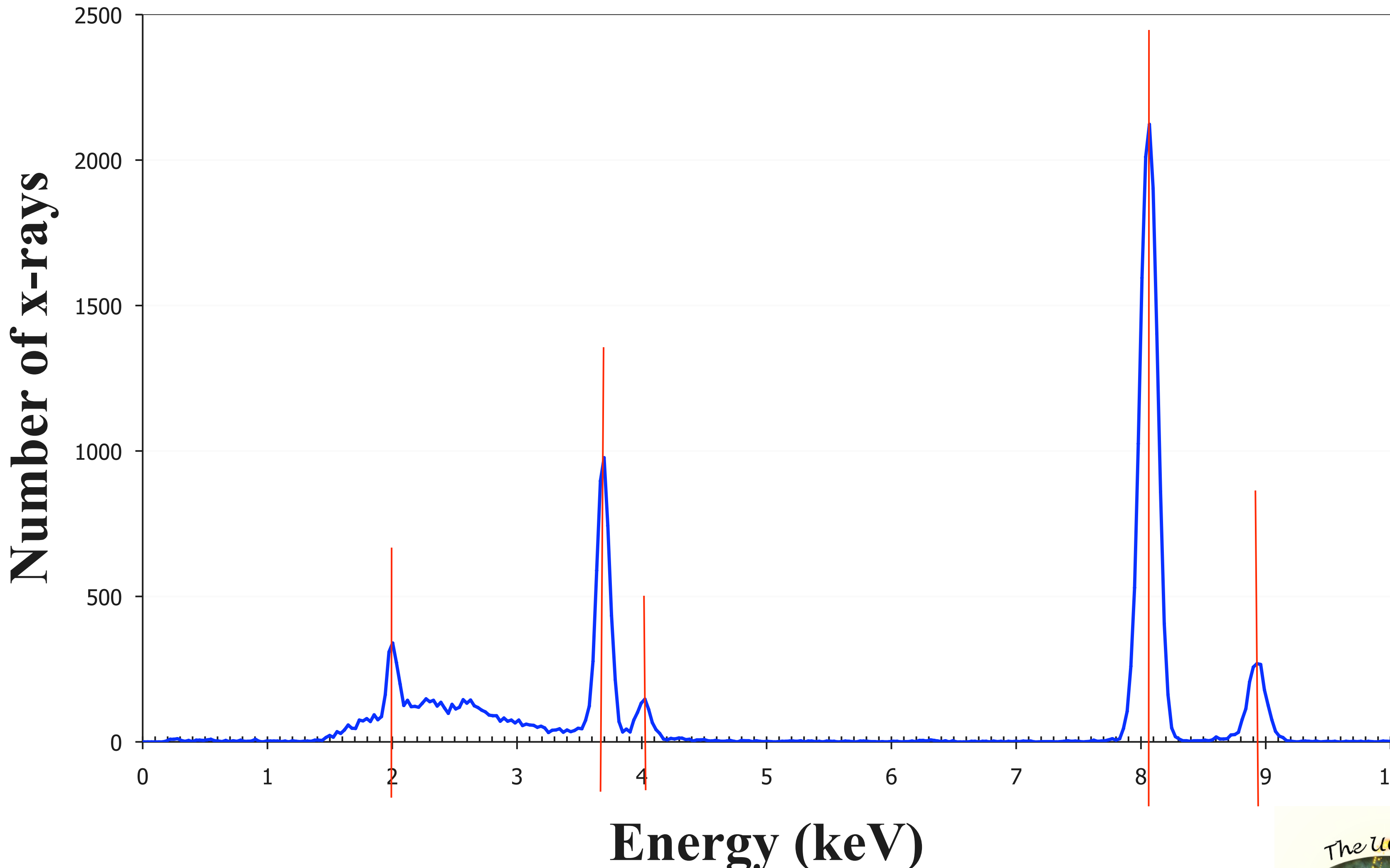
A typical *PIXE* Spectrum



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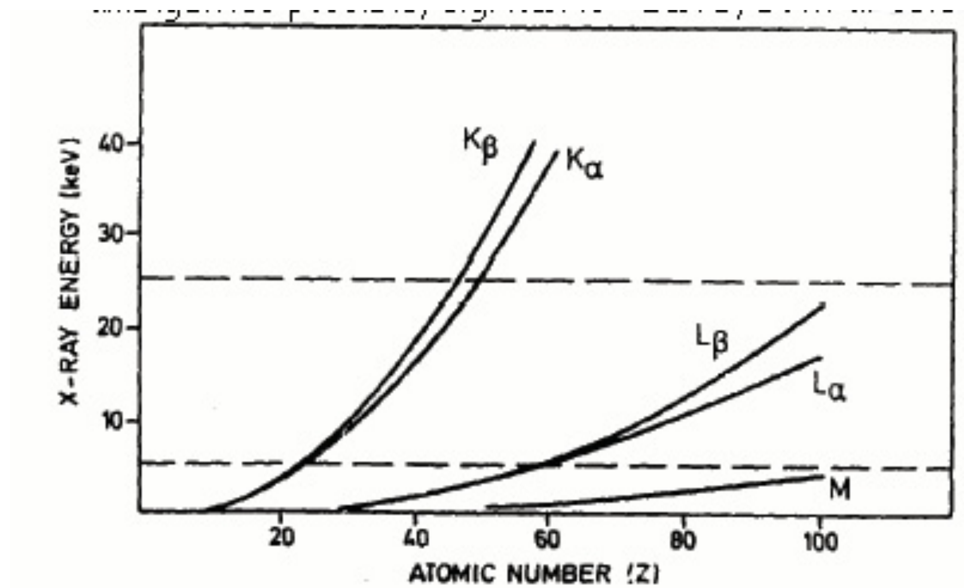
Characteristic X-ray production

• When a vacancy is created in the K shell, an electron in the L shell feels an effective charge of *(Z-1)e*$^-$. This is due to the *Ze*$^-$ charge of the nucleus and the *e*$^-$ remaining in the K shell. Thus the net force on an L shell electron is towards the K shell and a de-excitation occurs.



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• The transition wavelengths are given by

$$\frac{1}{\lambda} = R(Z-1)^2\left(\frac{1}{n_{lower}^2} - \frac{1}{n_{upper}^2}\right)$$

• The energy of the emitted x-ray is given by the Einstein relation: $E_{x-ray} = hf = \frac{hc}{\lambda} = hcR(Z-1)^2\left(\frac{1}{n_{lower}^2} - \frac{1}{n_{upper}^2}\right)$

The x-ray energies go as (*Z – 1*)^2 which produces the parabolic energy curves.

Comments: Derivation of the Bohr Theory

- **Energies and wavelengths are based on the Bohr Theory of the atom for an electron orbiting around a nucleus of charge Ze^-.**

$$F_{\text{centripetal}} = F_{\text{electrostatic}} \rightarrow \frac{m_e v_e^2}{r_e} = \frac{Ze^2}{4\pi\varepsilon_0 r_e^2} \rightarrow v_e^2 = \frac{Ze^2}{4\pi\varepsilon_0 m_e r_e}$$

- **Using the fact that the angular momentum of the electron $L = mv_e r_e$, we can write the above as**

$$v_n = \frac{Ze^2}{4\pi\varepsilon_0 L}$$

- **The angular momentum can also be represented as an integer multiple of Planck's constant, or the angular momentum is quantized.**

$$L = n\hbar = n\frac{h}{2\pi}$$

- **This is a completely non-classical result.**

• **Therefore the velocities are quantized, meaning they only have certain allowed values.**

$$v_n = \frac{Ze^2}{4\pi\varepsilon_0 n\hbar}$$

• **Now, returning to angular momentum, we can express the orbital radius in terms of this velocity that we just found.**

$$L = n\hbar = mv_n r_n \rightarrow r_n = \frac{n\hbar}{mv_n} = \frac{4\pi\varepsilon_0 n^2\hbar^2}{mZe^2}$$

• **The orbital radius is thus also quantized.**

• **If we have, for example, hydrogen with *Z = 1*, the radius of the 1st orbital, known as the *Bohr radius*, is given as**

$$r_1 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

• **Substituting the values of the constants gives the value of the Bohr radius**

$$r_1 = \frac{4\pi\left(8.85\times10^{-12}\,\frac{C^2}{Nm^2}\right)\left(\frac{6.63\times10^{-34}\,Js}{2\pi}\right)^2}{9.11\times10^{-31}\,kg\times\left(1.6\times10^{-19}\,C\right)^2} = 5.31\times10^{-11}\,m$$

- **One more thing about orbital radii…**

$$r_n = \frac{4\pi\varepsilon_0 n^2\hbar^2}{mZe^2} = n^2 r_1$$

- **The radius of the n^th orbital can be expressed as an integer multiple of the Bohr radius.**

- **Now, this is nice and all, but we really want to be able to calculate the energy of individual orbits and then talk about differences in energy levels.**

- **This will allow us to talk about the x rays emitted when an electron transitions between an upper orbital and a lower orbital.**

- **So, how do I calculate the energy of any orbital?**

- **The energy of an orbit is the sum of the kinetic energy of the electron and a potential energy due to its position with respect to the nucleus.**

The potential energy of a particle of mass m and charge –*e* a distance *r* from a heavy nucleus of charge +*Ze* is given as

$$V_n = -\frac{Ze^2}{4\pi\varepsilon_0 r_n}$$

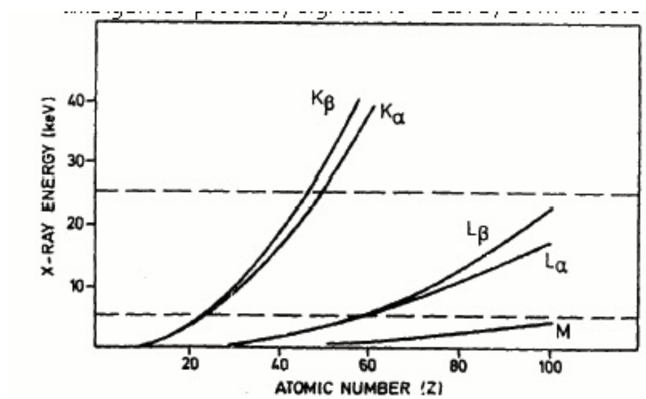
The energy of the orbit is given as

$$E = \frac{1}{2}mv_n^2 + V_n = \frac{1}{2}m\left(\frac{Ze^2}{4\pi\varepsilon_0 n\hbar}\right)^2 - \frac{Ze^2}{4\pi\varepsilon_0 \dfrac{4\pi\varepsilon_0 n^2\hbar^2}{mZe^2}}$$

Doing the math…

$$E_n = -\frac{Z^2 me^4}{2(4\pi\varepsilon_0)^2 n^2\hbar^2}$$

And here we are, the energy of the nth orbital for a *hydrogen-like* (*1 electron*) atom.



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Notice that the energy is proportional to *Z^2* and if you plot the energy versus atomic number you get parabolic energy curves.

The X-ray Energies

The energies of an emitted x-ray are given as the difference between where the electron originates and where the electron is going to

$$\Delta E = E_{upper} - E_{lower}$$

So we have:

$$\Delta E = E_{upper} - E_{lower} = -\frac{Z^2 m e^4}{2(4\pi\varepsilon_0)^2 n_{upper}^2 \hbar^2} - \left(-\frac{Z^2 m e^4}{2(4\pi\varepsilon_0)^2 n_{lower}^2 \hbar^2}\right)$$

$$\Delta E = \frac{Z^2 m e^4}{2(4\pi\varepsilon_0)^2 \hbar^2}\left(\frac{1}{n_{lower}^2} - \frac{1}{n_{upper}^2}\right) = hf = \frac{hc}{\lambda}$$

On Wednesday we'll examine this formula and see what it tells us…..

In particular we'll calculate the K_α and K_β transition energies of a particular element.

Then we'll discuss how well our results agree with experiments and look at a *PIXE* spectrum for a single element