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 (*ERDA*)
    - 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* & ERDA

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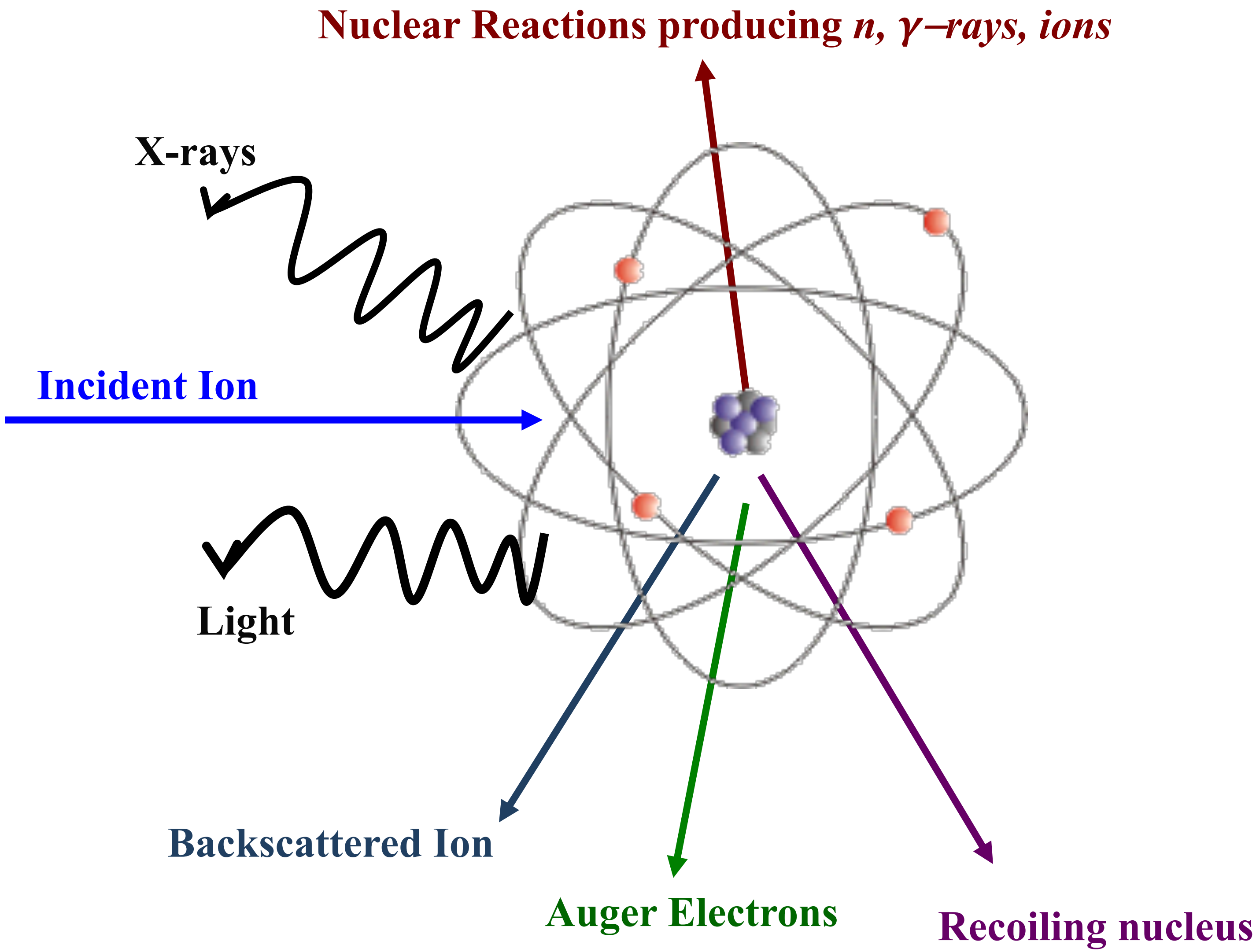
Introduction: Ion –Target Interaction



Proton Induced X-ray Emission Spectroscopy

PIXE

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

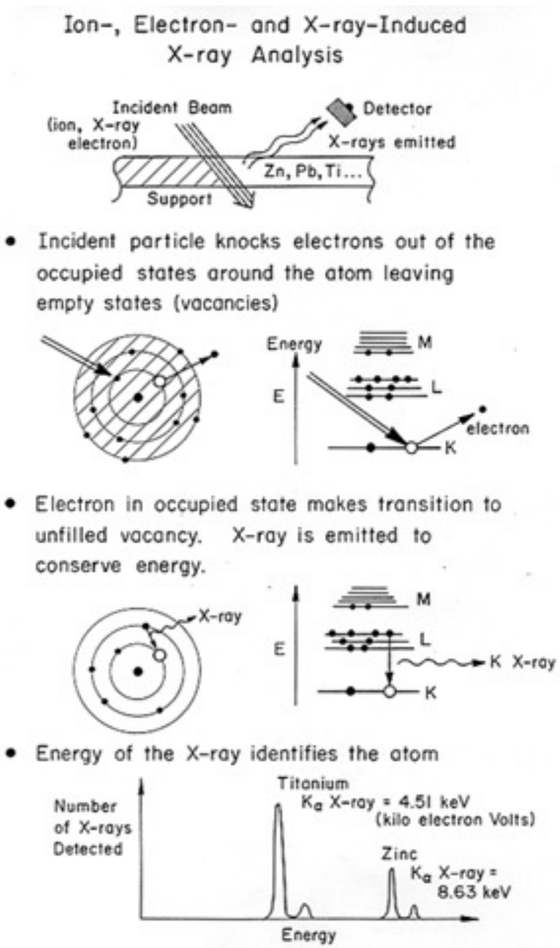
- X-ray emission induced by charged particles from a radioactive source. We're going to produce protons on our accelerator and shoot them at a target to produce x-rays.

- 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

- 2022: most widely used technique in materials analysis, atmospheric aerosols, archaeology, paleontology, archaeometry, criminology, biology, geology, environmental sciences.....

PIXE: The Basics



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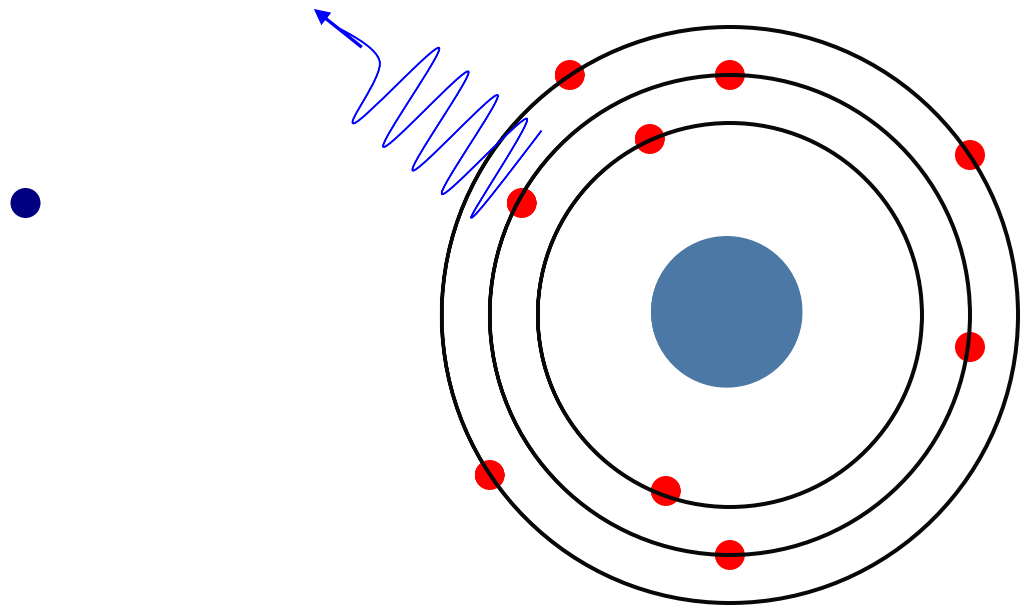
- Incident proton interacts with electrons in the material ejecting electrons.
- This creates a vacancy in a shell that is usually filled with an electron from a higher orbit.
- For the electron to fill this vacancy it needs to lose energy.
- The energy difference is the difference from where the electron 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.

An Illustration of the *PIXE* process



L_{α} transition in an atom

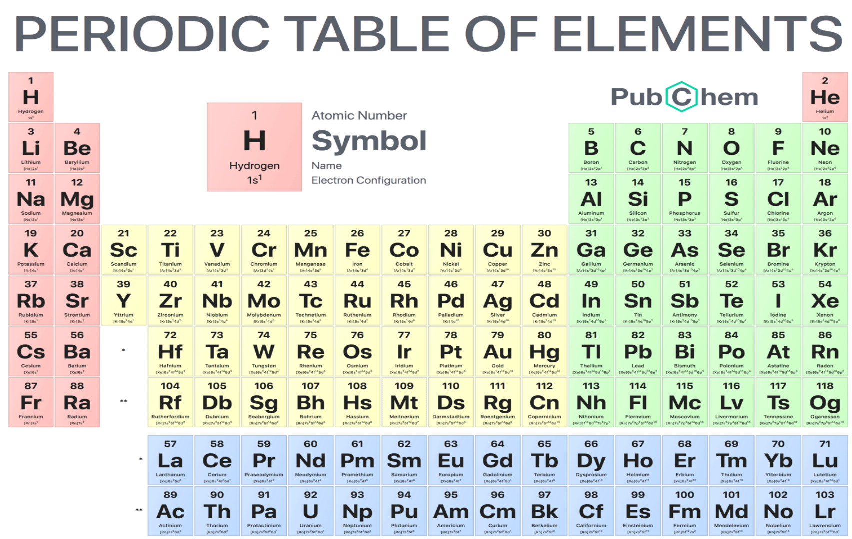
The incident proton ejects an electron from the $n = 2$ orbital and creates a vacancy in the $n = 2$ orbital. An electron from the $n = 3$ orbital de-excites to fill the vacancy created in the $n = 2$ orbital and emitting an x-ray in the process that we can detect.

PIXE: The Basics

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

- Heavier elements (greater than $Z = 50$) are measured through their *L shell* X rays because the beam energy is not enough to eject the tightly bound *K shell* electrons.

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



Characteristic X-ray production

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

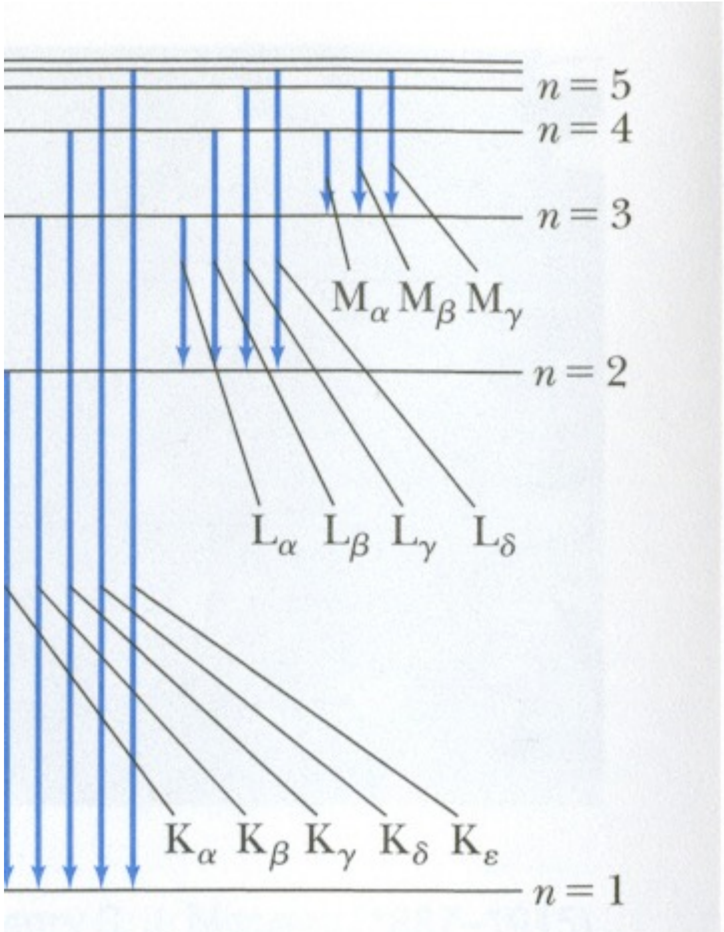
• The energy of the photon emitted depends on the energy of the upper state (E_{upper}) and the energy of the lower state (E_{lower}).

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

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

• The actual energies are determined from the Schrodinger equation of quantum mechanics.

•We need to determine a formula for the upper and lower energy states.



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

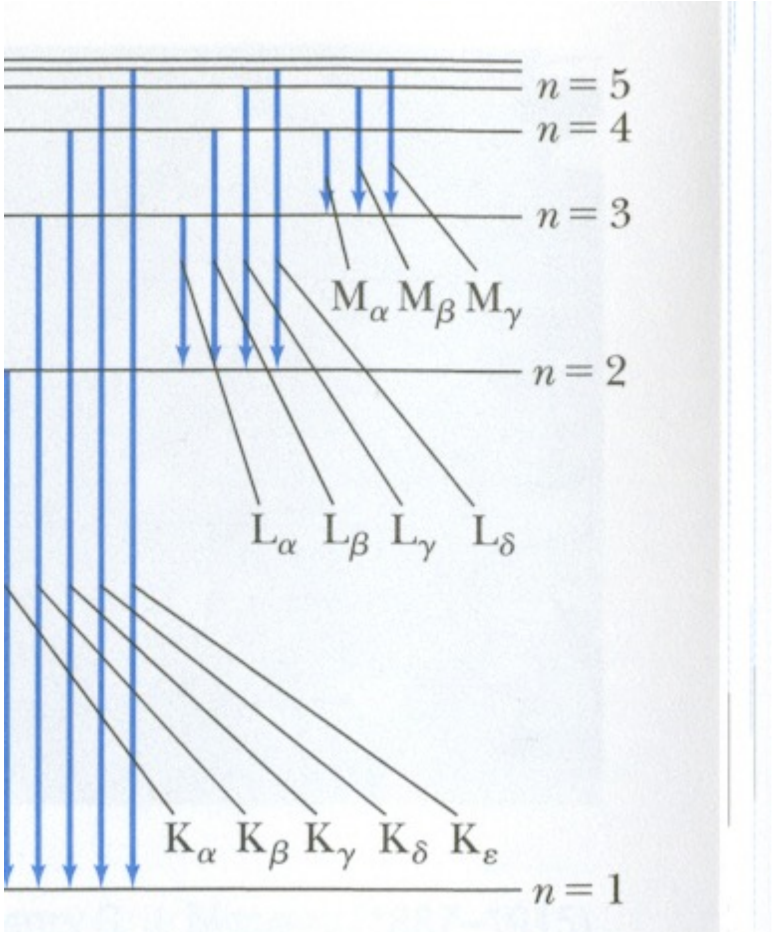
Characteristic X-ray production

- 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 atomic number and the frequency of the x-ray emitted (or the energy of the x-ray emitted as is how we will use it). Plots like those on the right are called Moseley Plots.

• This is the most fundamental idea behind PIXE.

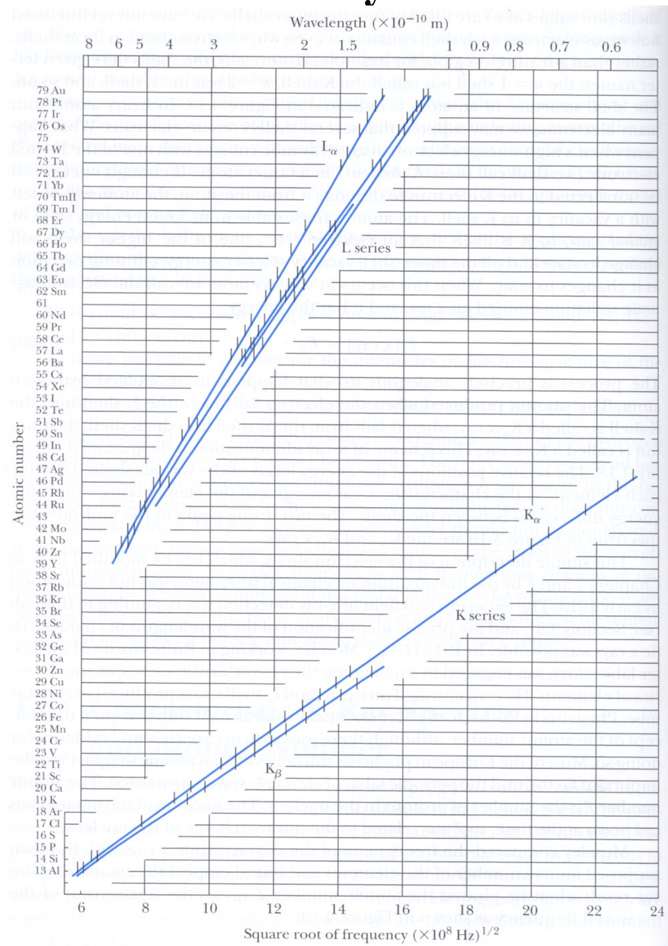
• It shows that for each atomic number (element) there are a characteristic set of x-ray wavelengths and energies emitted.

• Moseley found the relationship to be of the form:

$$Z = a\sqrt{f} + b$$

where a and b are constants from the fitting of a line to the data.

Moseley Plots



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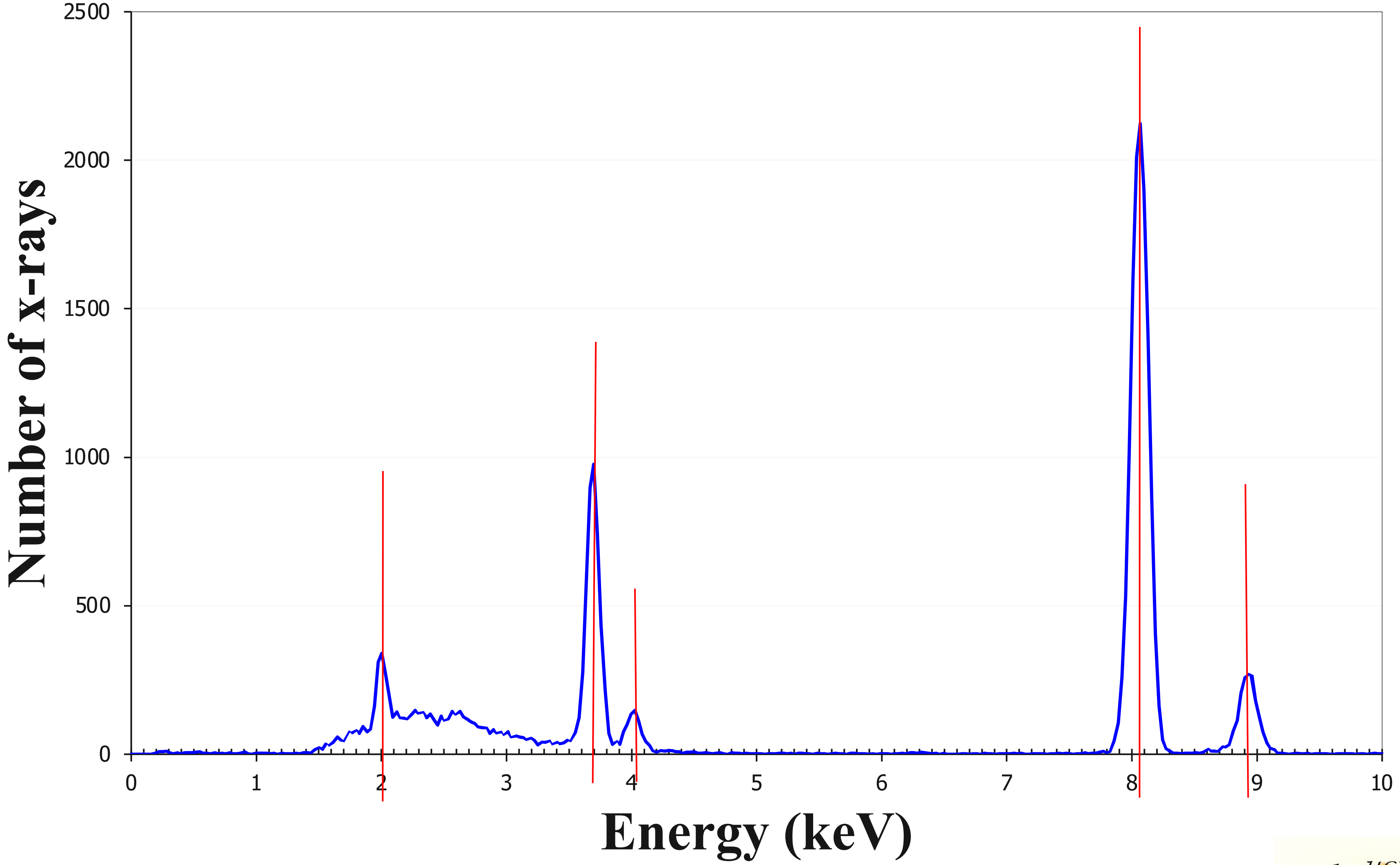
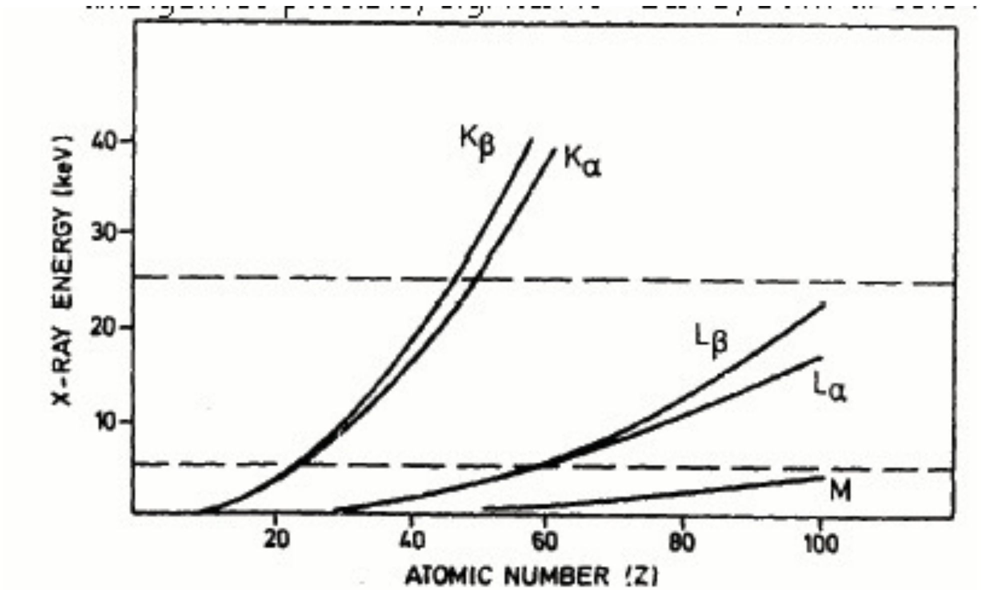
A typical *PIXE* Spectrum



Characteristic X-ray production

• When a vacancy is created in the K shell ($n = 1$ orbital), an electron in the L shell ($n = 2$ orbital) 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 energies are given by the Einstein relation

$$\Delta E_{photon} = E_{x-ray} = hf \approx -13.57eV\left(\frac{1}{n_{lower}^2} - \frac{1}{n_{upper}^2}\right)Z^2$$

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

- Notice that if we rearrange the above equation and take a square root, we get the form that Moseley obtained, namely:

$$Z = a\sqrt{f} + b$$

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 or quantum mechanical 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

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

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- 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.

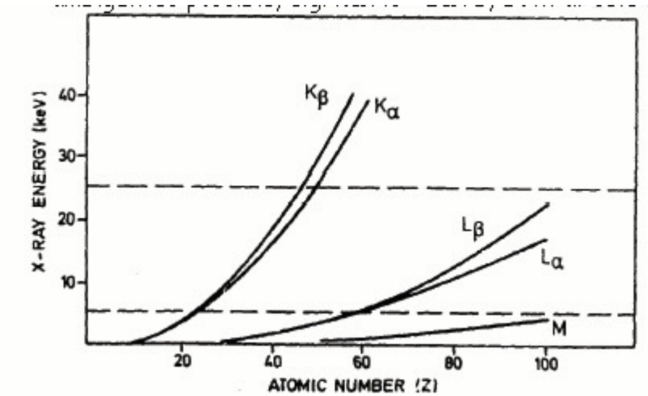
- This will allow us to talk about the x-rays emitted when an electron transitions between an upper orbital and a lower orbital.

- 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

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



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

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

- Notice that the energy is proportional to Z^2 and if you plot the energy versus atomic number, you get parabolic energy curves which is what Moseley obtained.

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:

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

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

$$\rightarrow \Delta E = -13.6eV\left(\frac{1}{n_{upper}^2} - \frac{1}{n_{lower}^2}\right)Z^2$$

- Next, we'll examine this formula and see what it tells us…..

- 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