X-Ray Fluorescence and Natural History

How XRF Helps

XRF can be used both quantitatively (homogenous samples) and quantitatively (heterogenous samples).

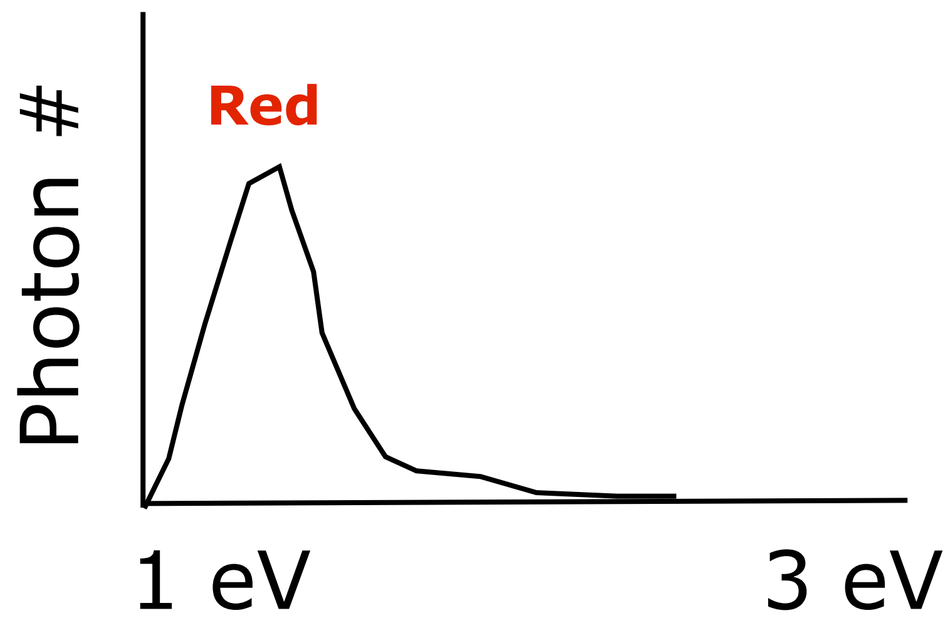
- Trace elements in a fossil can help identify source, or give insight into diagenetic processes
- Chemostratigraphic profiles can help understand formation processes and paleoenvironments
- In curation contexts, elemental data can help with conservation decisions (specifically regarding arsenic, uranium, lead, etc.)

How we see color

Color is fundamentally a fluorescence process:

- a **photon** is emitted from a source
- The emitted **photon** interacts with the molecules in the sample
- Based on the properties of the molecule, the **photon** is either reflected back, scattered, or absorbed.
- Our eyes see the reflected photon through our cone cells and send the information to a processor (our minds) which perceive color.

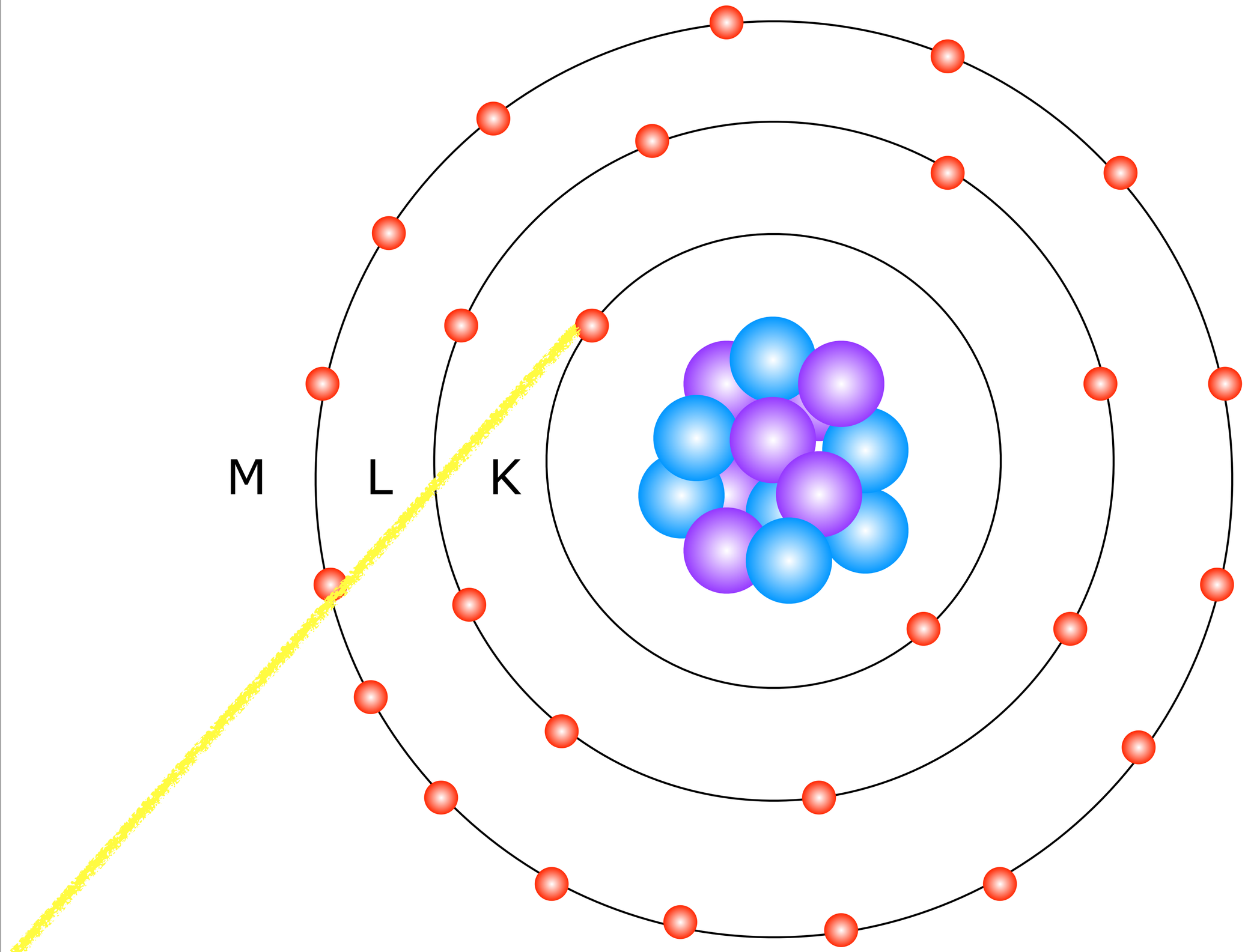
- **Red** is 1 eV
- **Violet** is 3 eV

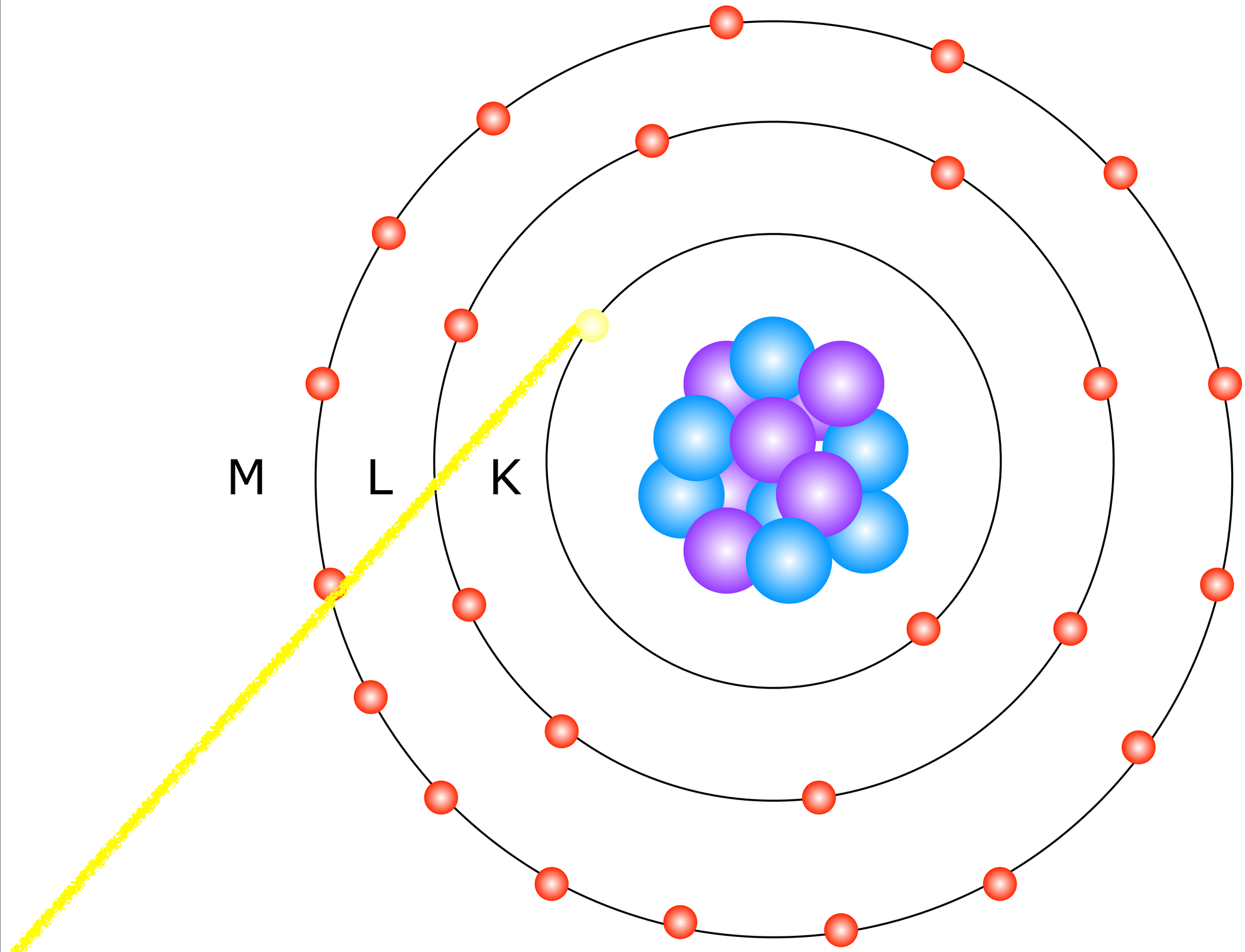


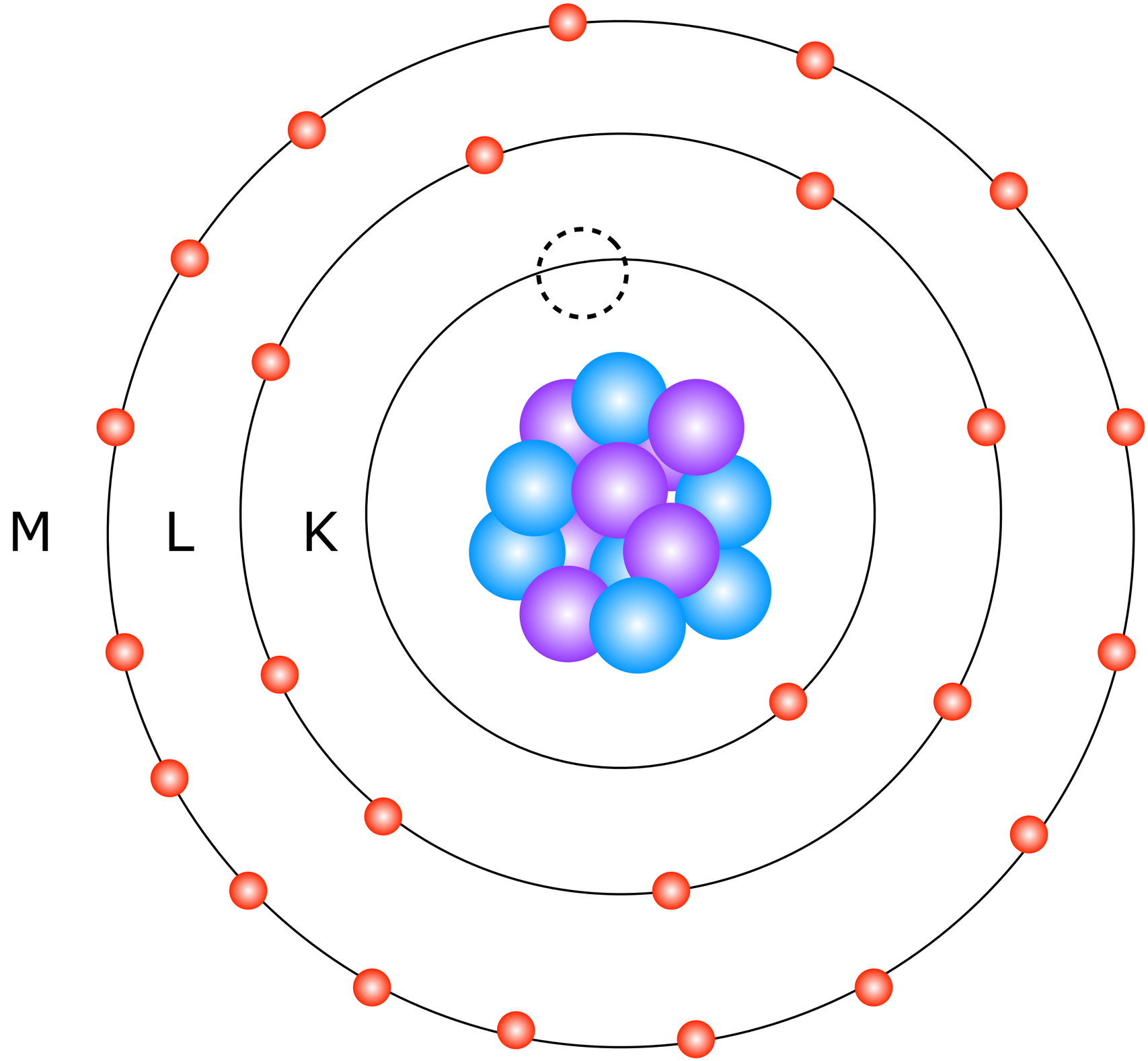
How it Works – What is x-ray fluorescence?

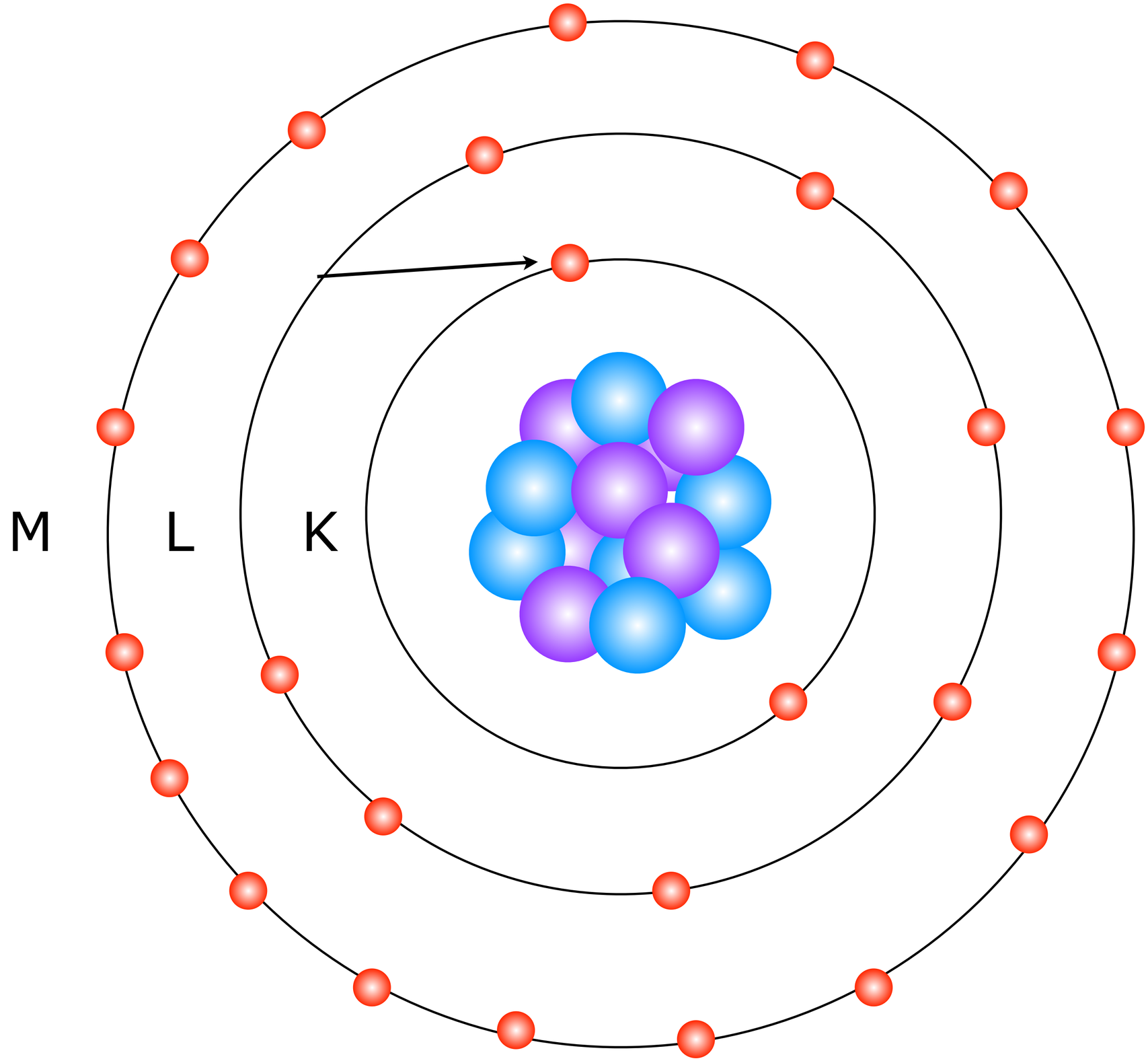
In the most basic terms, x-ray fluorescence is the process in which:

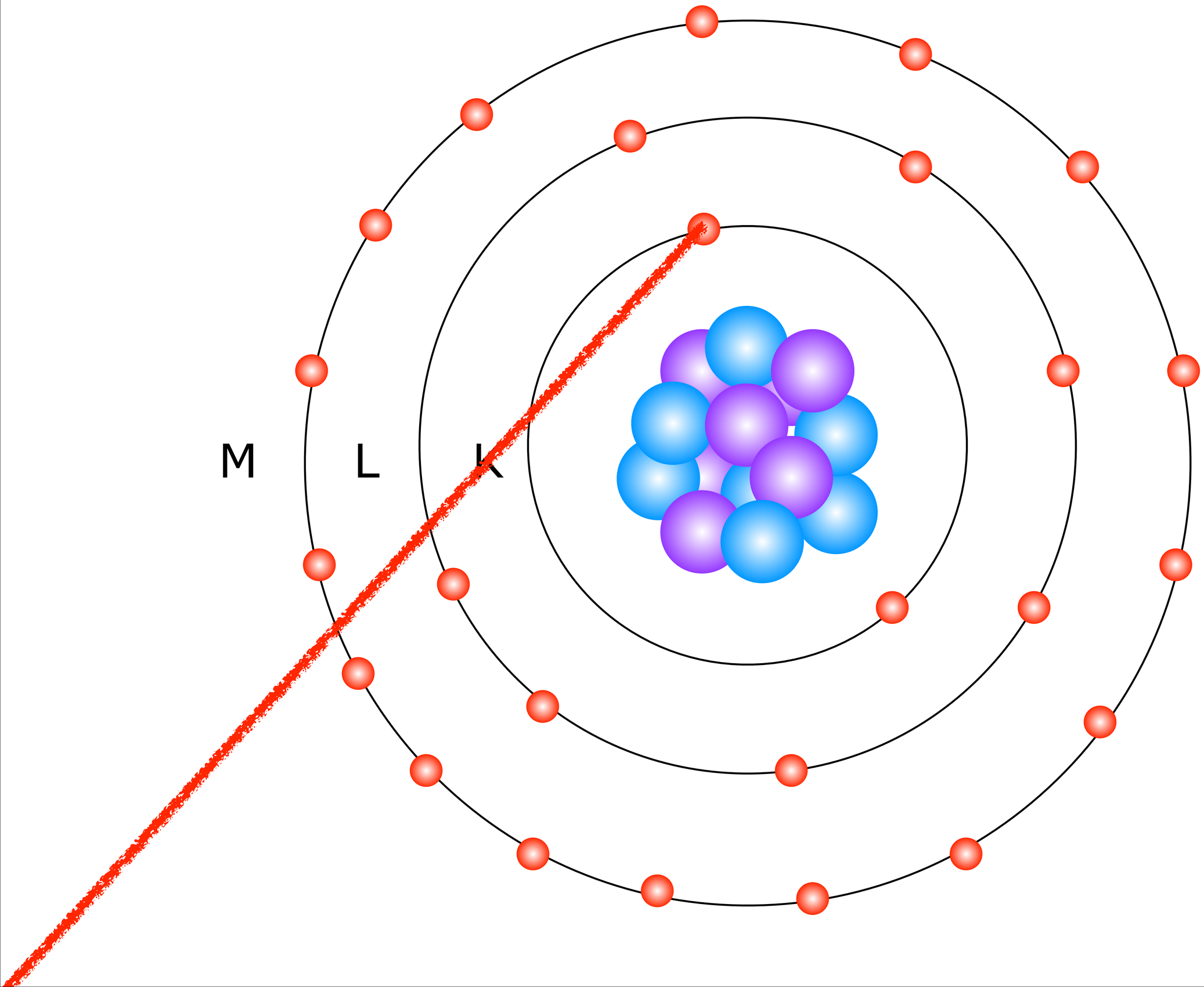
- a **photon** is emitted from an x-ray source
- The emitted **photon** interacts with the atoms in the sample
- In some cases, this interaction causes an electron to get "knocked out" of the inner shell of a given atom
- When an electron leaves an inner shell, the atom becomes "unstable" and wants to fill the vacancy, so an electron from a higher shell drops down to fill that vacancy
- When an electron drops from a higher to a lower shell, a certain energy is released in the form of another **photon**, which is characteristic not only to each element, but to each shell transition; this is fluorescence
- In x-ray fluorescence instruments, a detector is used to pick up the characteristic fluorescent energies.

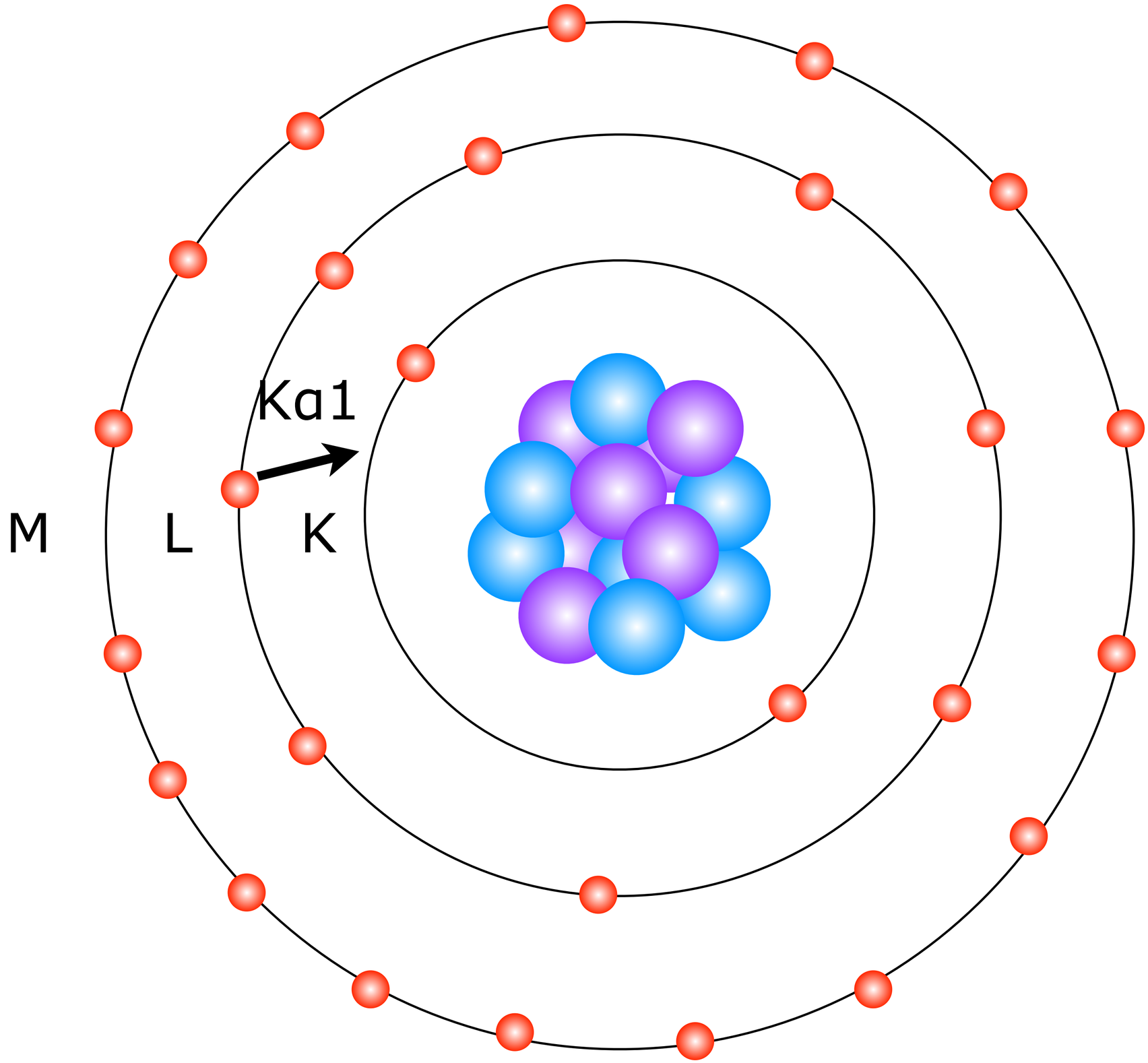

M
L
K

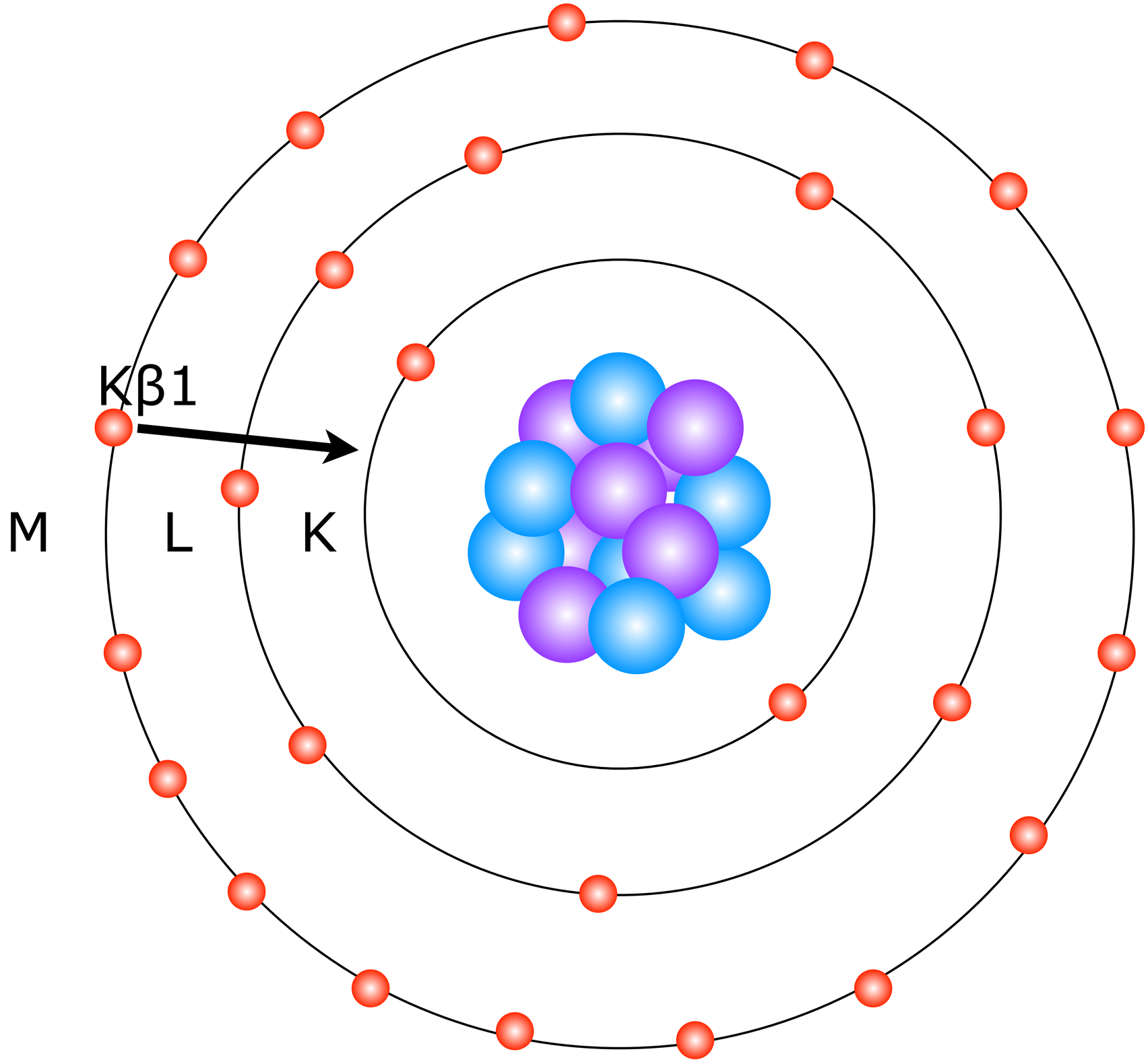

M
L
K


M
L
K

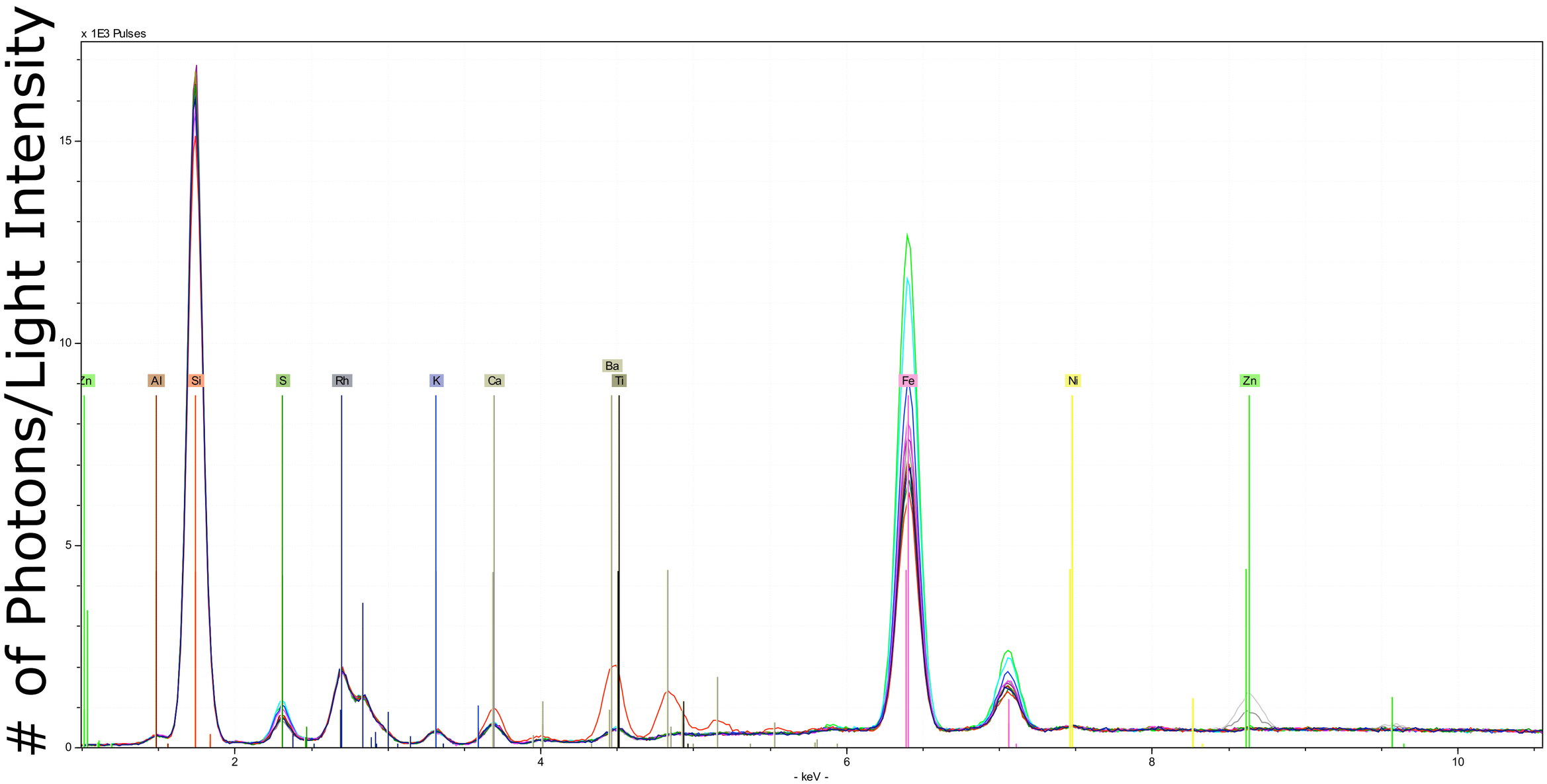

M
L
K


M
L
K


Kα1
M
L
K


Kβ1
M
L
K

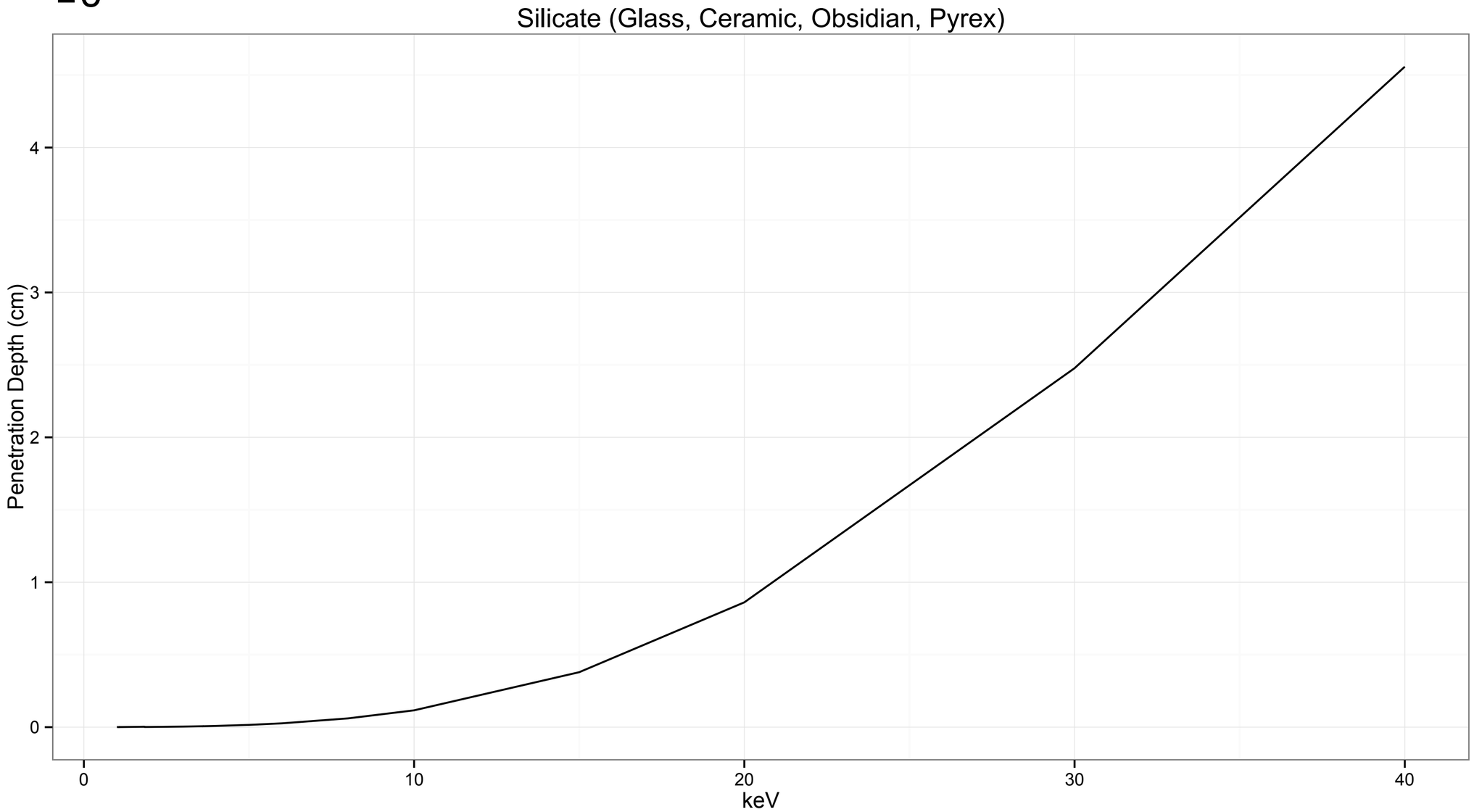
Analysis of Spectra



The x axis shows increasing energy - each element ‘lights up’ at a different and unique energy

How deep can we measure? Silicates

$$\frac{I}{I_0} = e^{(-\mu/\rho)x}$$



As you go up in energy, you analyze deeper within the artifact

How deep can we measure? Ceramics

Element	Photon Emitted energy (keV)	Analysis depth in Ceramic(cm)
O	0.53	0.000001
Na	1.04	0.0007
Mg	1.2	0.00096
Al	1.47	0.0017
Si	1.74	0.0027
P	2.01	0.0013
Ca	3.69	0.0064
Cr	5.41	0.0192
Fe	6.4	0.03
Cu	8.01	0.058
Zn	8.64	0.077
Pb	10.55	0.113
Zr	15.78	0.384

The 5 Parameters for Data Collection

1. The same energy (in keV)
2. The same current (in μA)
3. The same filter
4. The same time of analysis
5. The same atmosphere (air, vacuum, etc.)

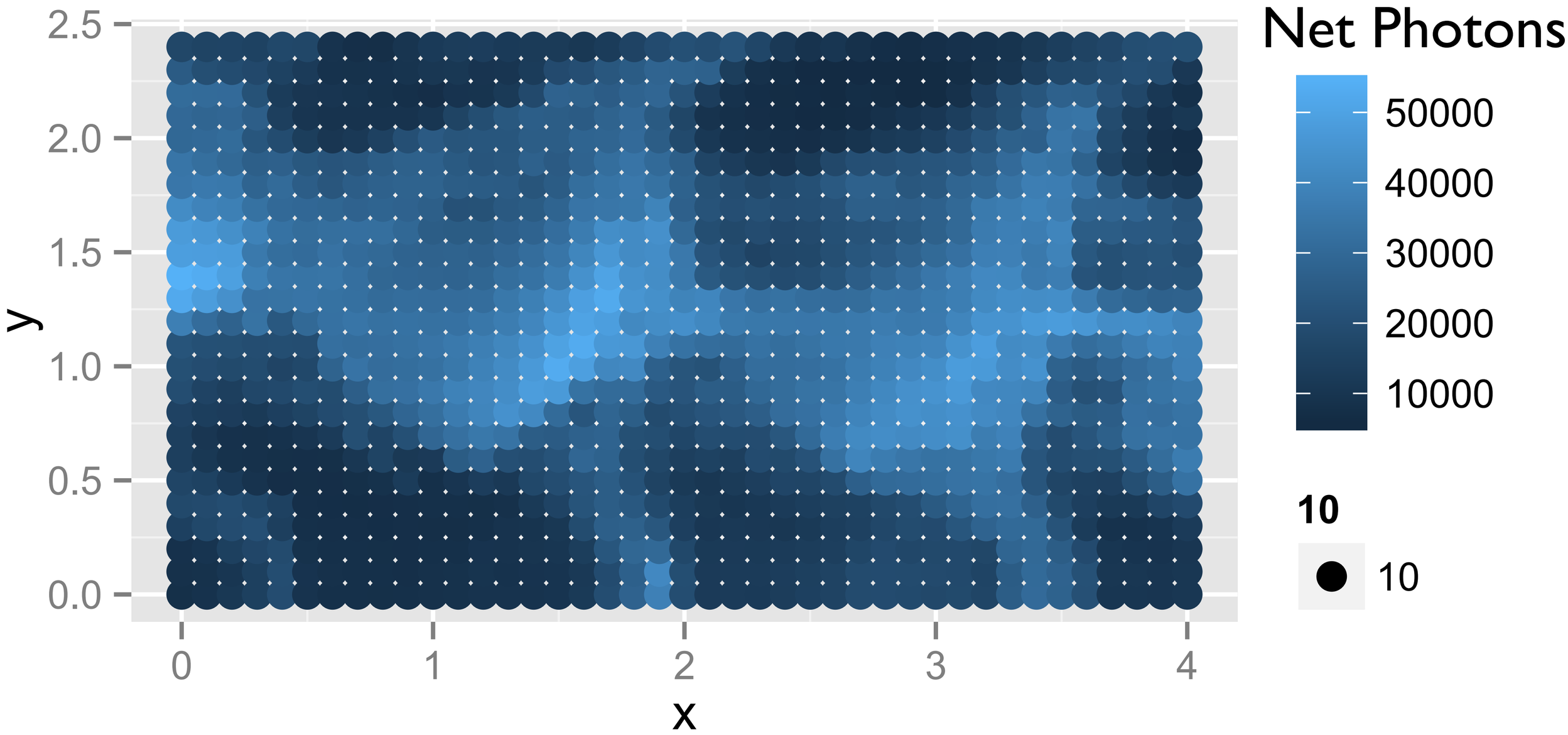
Imaging with XRF

XRF can be used to create elemental images

- A simple color ramp can be used to show high and low concentrations of elements
- False-color images can be generated when red, green, or blue is assigned to different elements

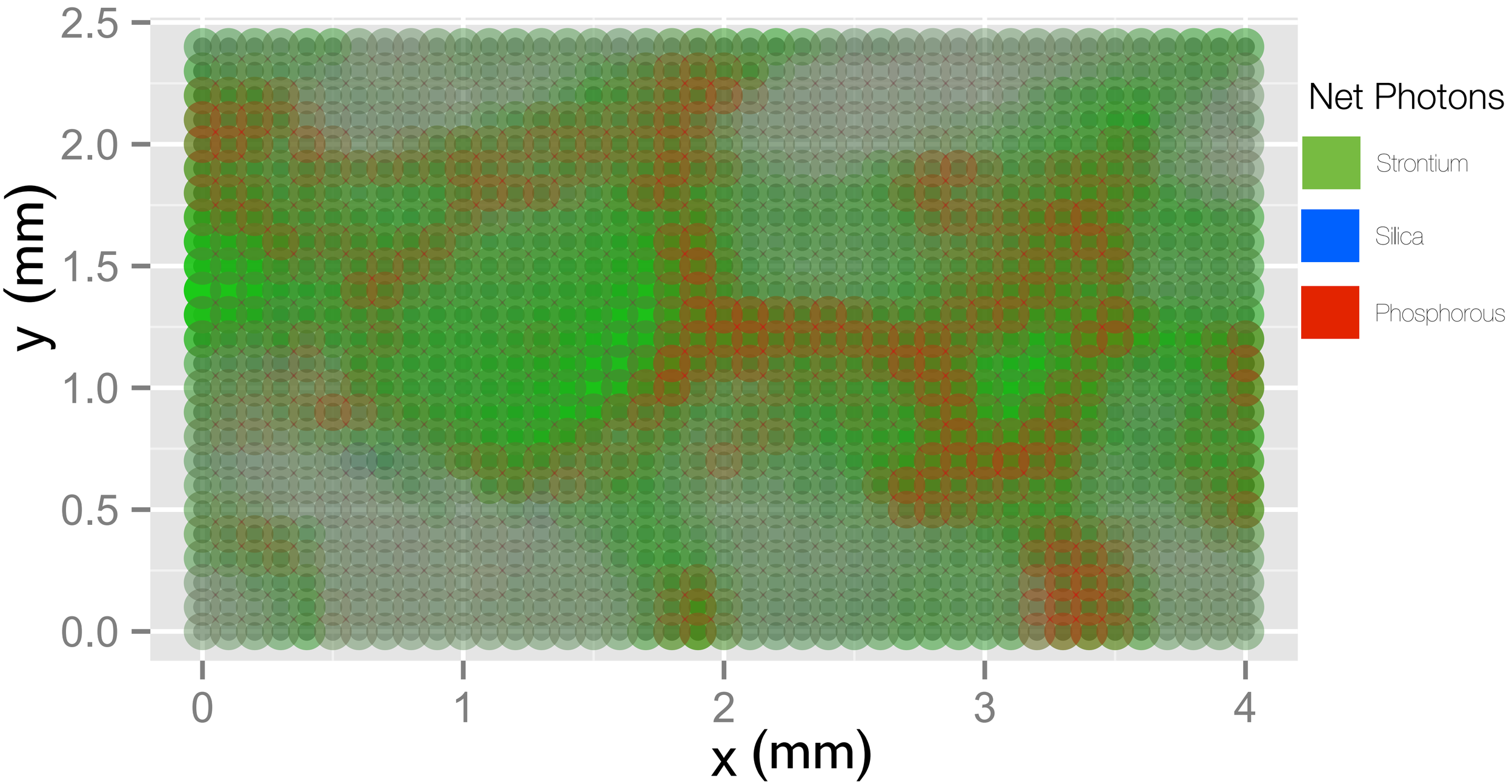
Fossil Fish from Green River Formation

Strontium Ka1 (14.16 keV)



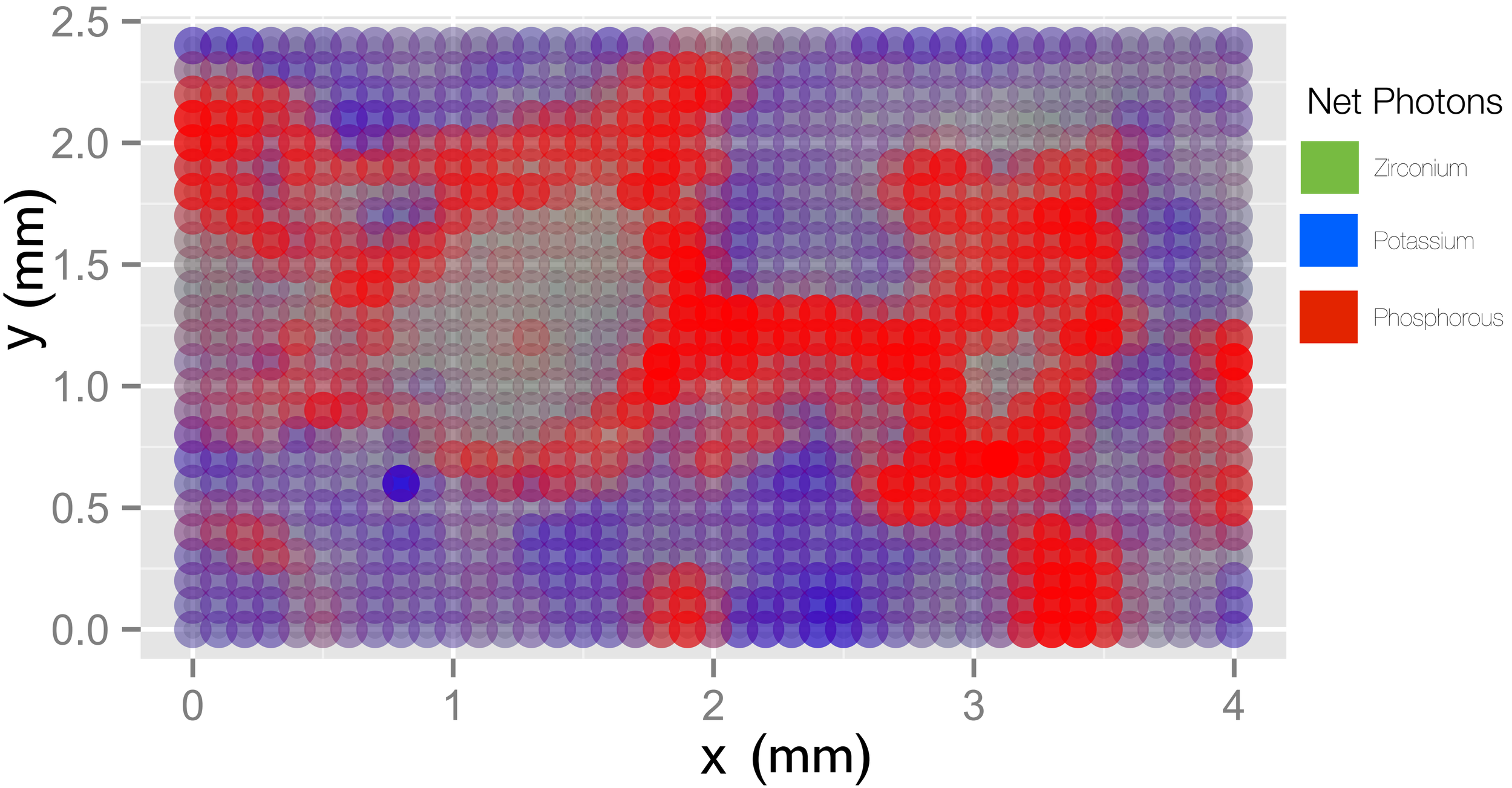
Fossil Fish from Green River Formation

Strontium, Silica, and Phosphorous Ka1

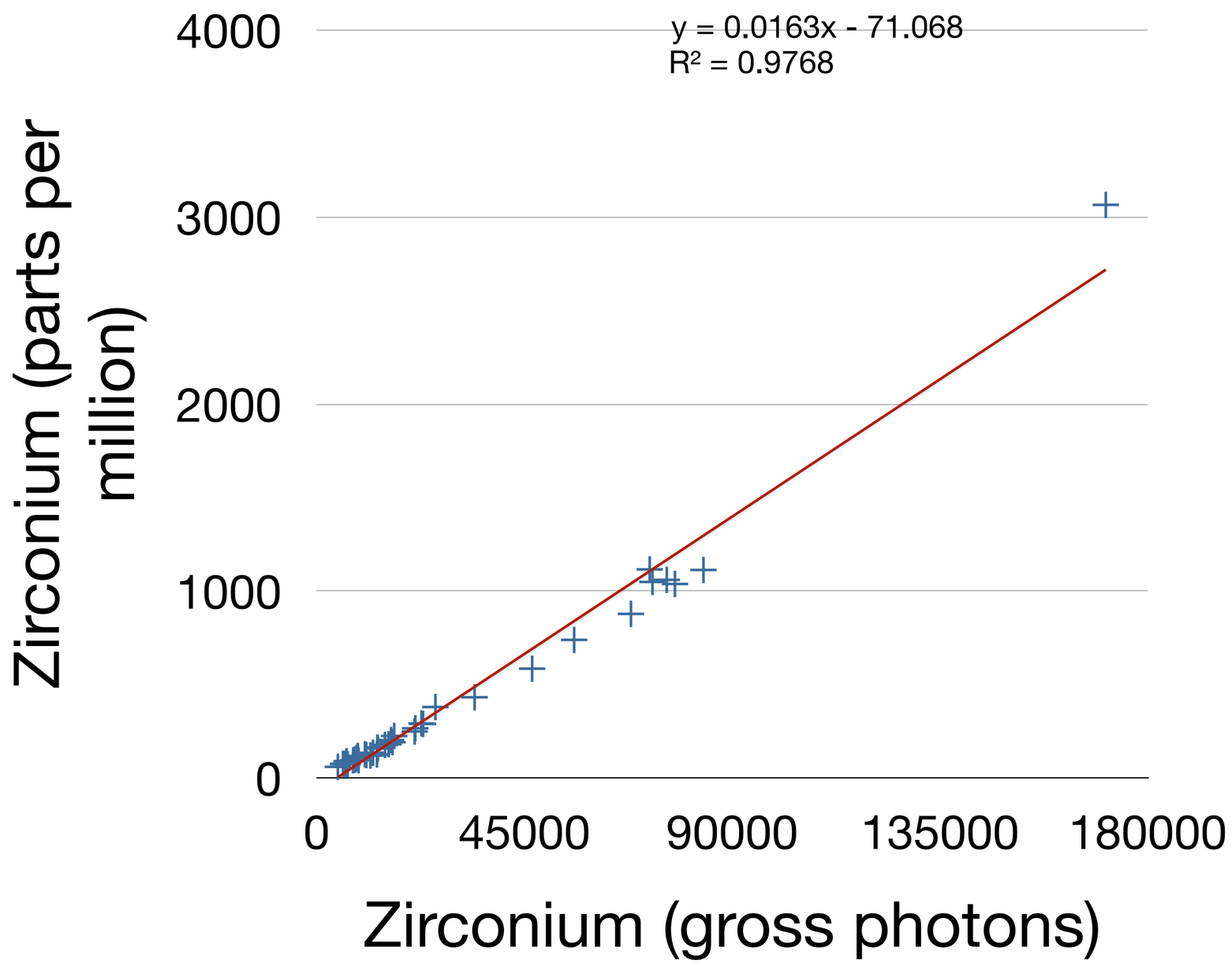


Fossil Fish from Green River Formation

Strontium, Silica, and Phosphorous Ka1



When to quantify results?



When to quantify results?

Quantification is a set of linear models/regressions

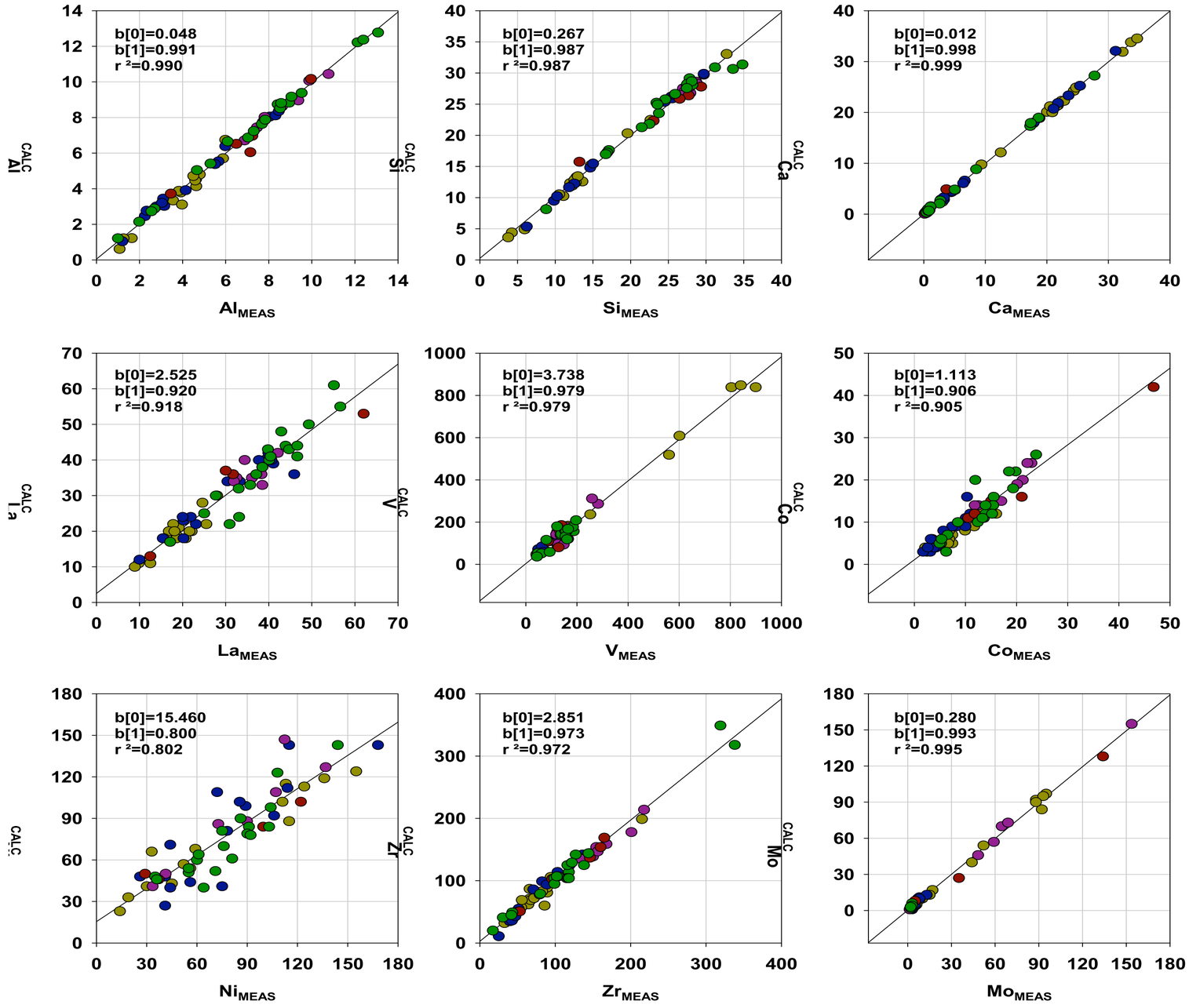
Lucas-Tooth and Price (1961) Equation:

$$C_i = r_0 + I_i[r_i + \Sigma(r_{in}I_n)]$$

In which C_i represents the concentrate of a given element of the sample in weight % or ppm, r_0 is the intercept/constant, r_i is the slope of photons for element i, r_{in} is the slope of photons for element n that influence the fluorescence of element i, I_i is the quantity of photons for element i, and I_n is the quantity of photons for element n.

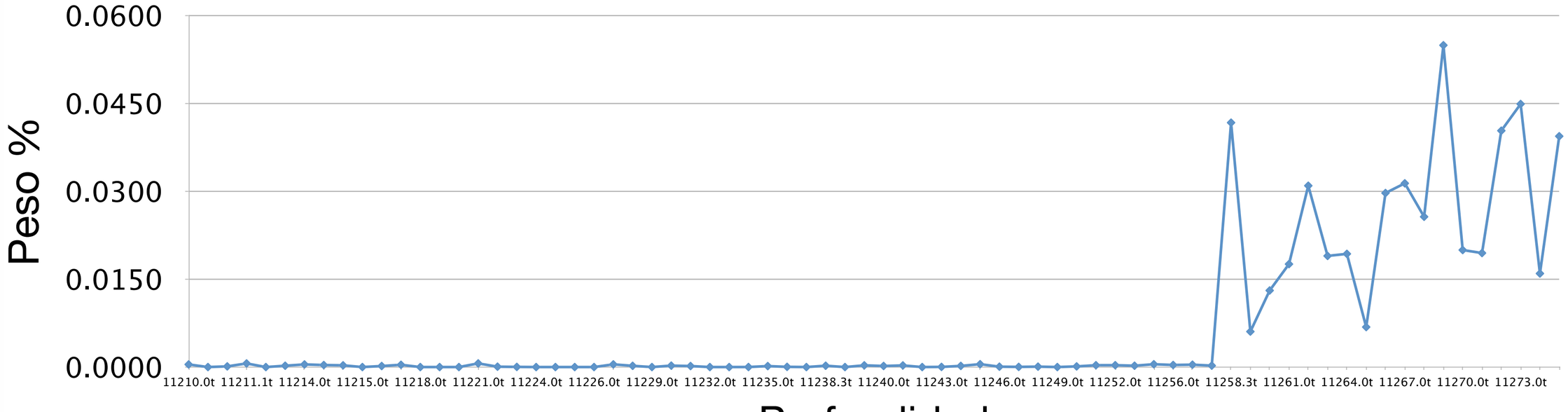
When to quantify results?

Quantification is basically a complicated set of linear models/regressions

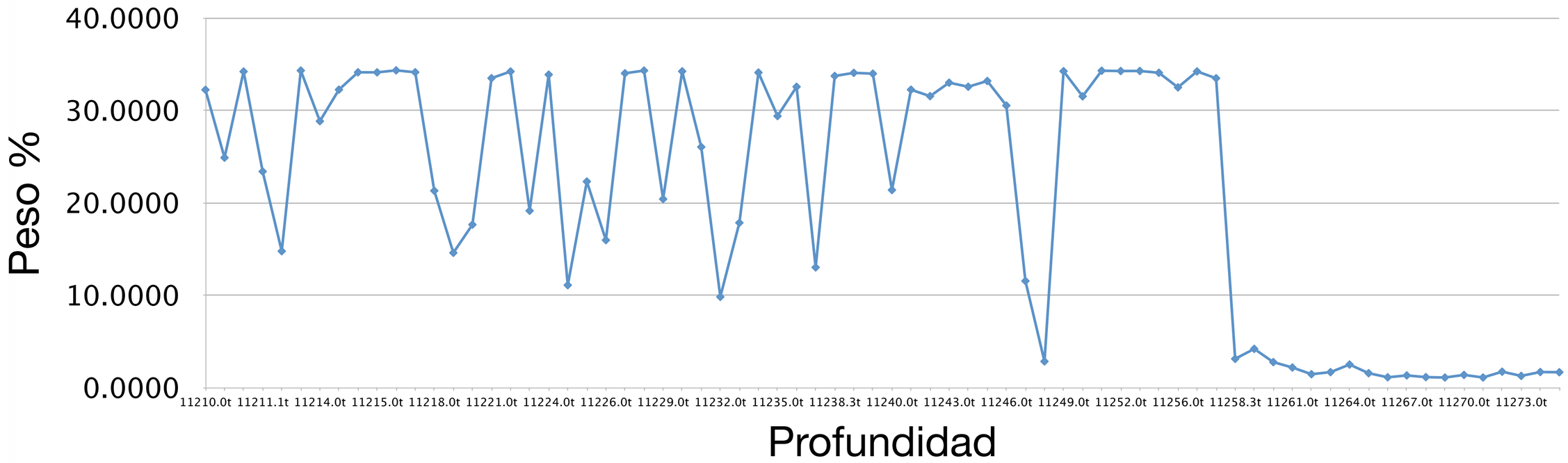


- Eagle Ford Shale
- Barnett Shale
- Ohio Shale
- Int'l Shale Standards
- Smithwick Shale

Molybedinum (Mo)



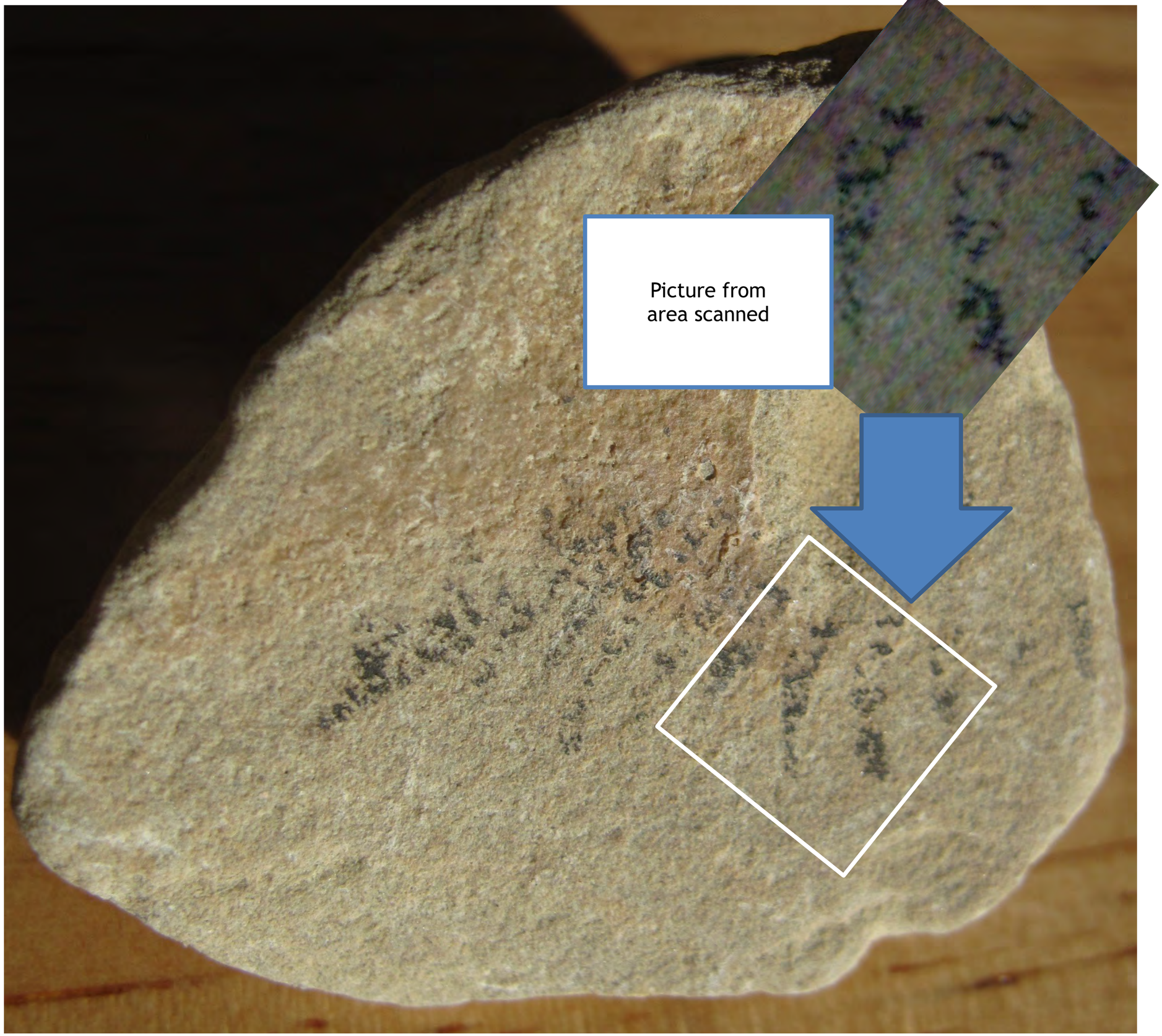
Calcium (Ca)



Quantitative and Qualitative XRF

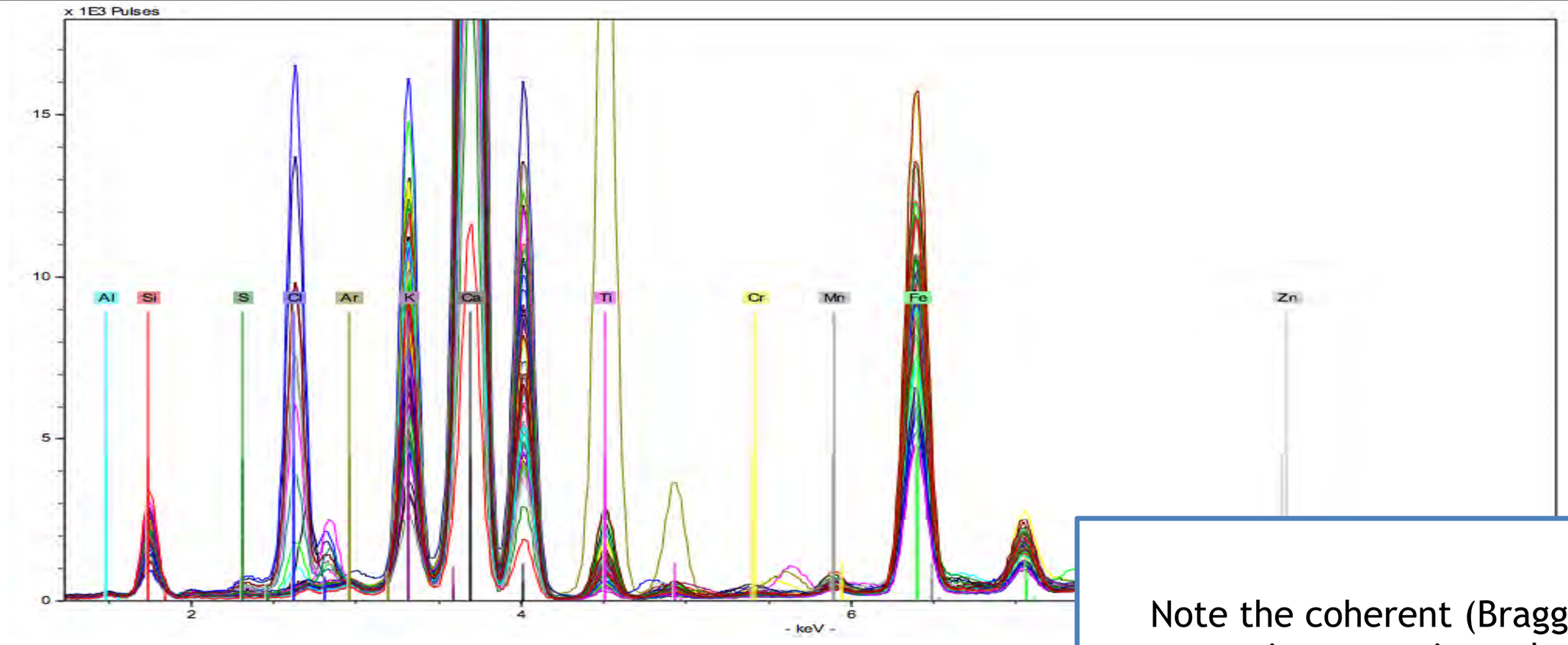
XRF can be used both quantitatively and qualitatively

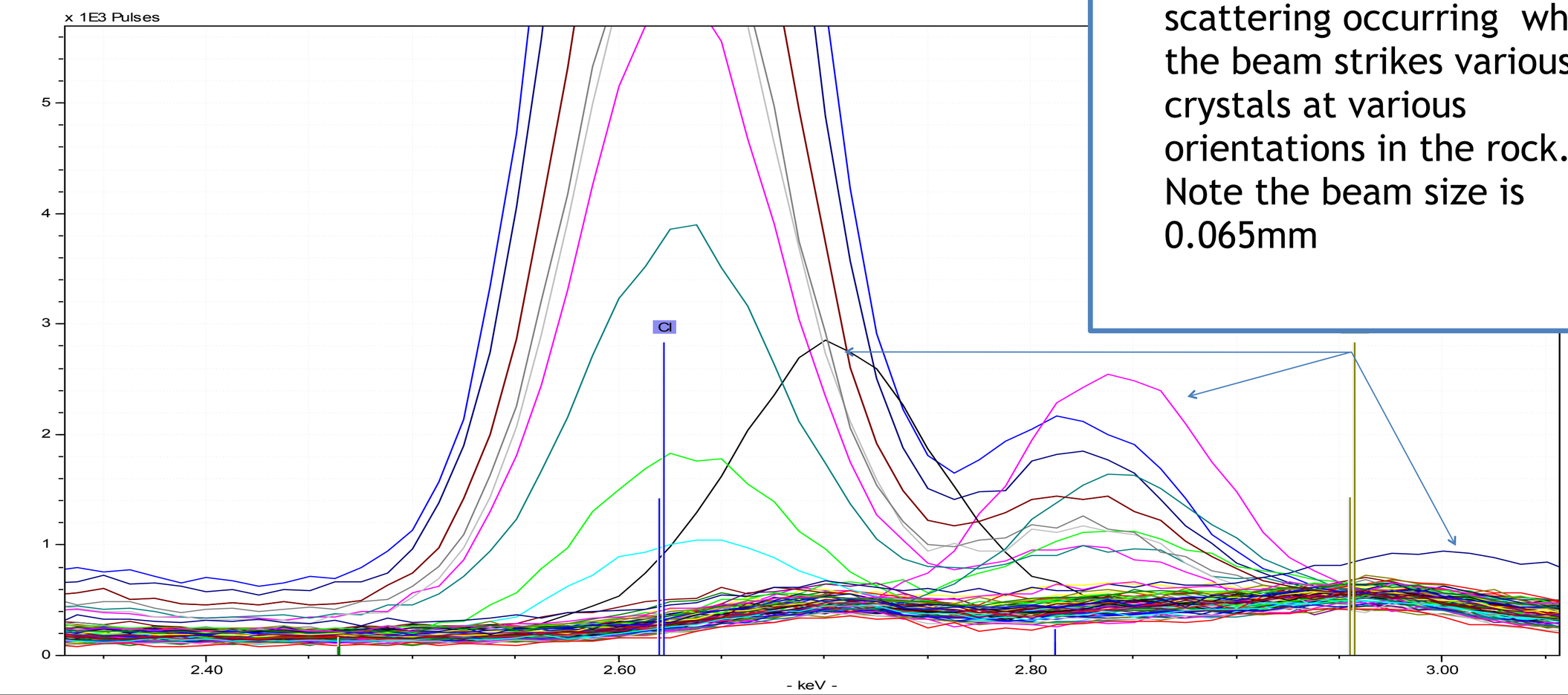
- While quantitative data can be collected from homogenous materials, qualitative data from heterogenous materials can be helpful as well


Picture from
area scanned

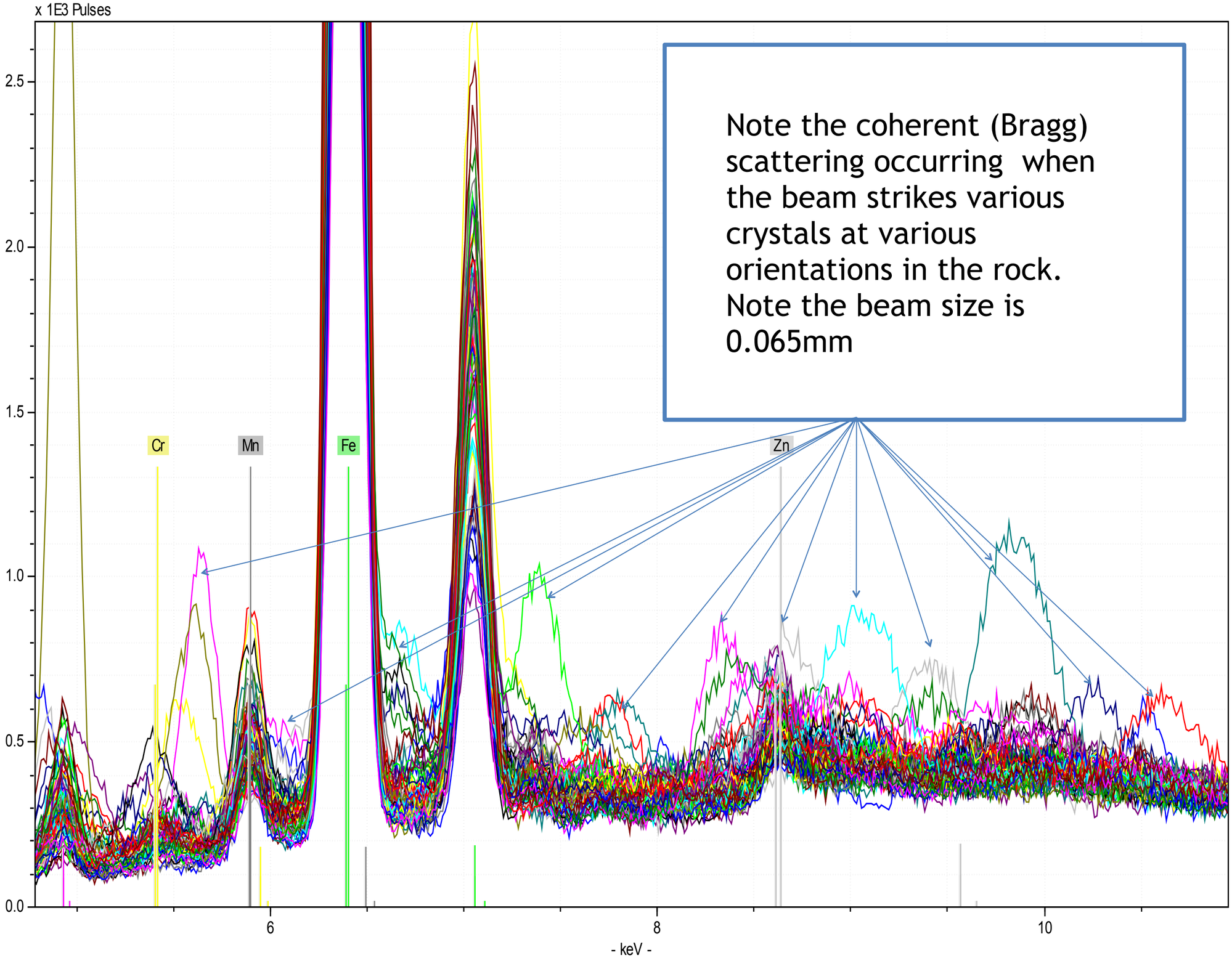
Spectra at various locations at various scales

Note the coherent (Bragg) scattering occurring when the beam strikes various crystals at various orientations in the rock
Note the beam size is 0.065mm





Note the coherent (Bragg) scattering occurring when the beam strikes various crystals at various orientations in the rock. Note the beam size is 0.065mm


x 1E3 Pulses
2.5
2.0
1.5
1.0
0.5
0.0
Cr
Mn
Fe
Zn
6
8
10
- keV -
Note the coherent (Bragg) scattering occurring when the beam strikes various crystals at various orientations in the rock. Note the beam size is 0.065mm