X-Ray Experiments

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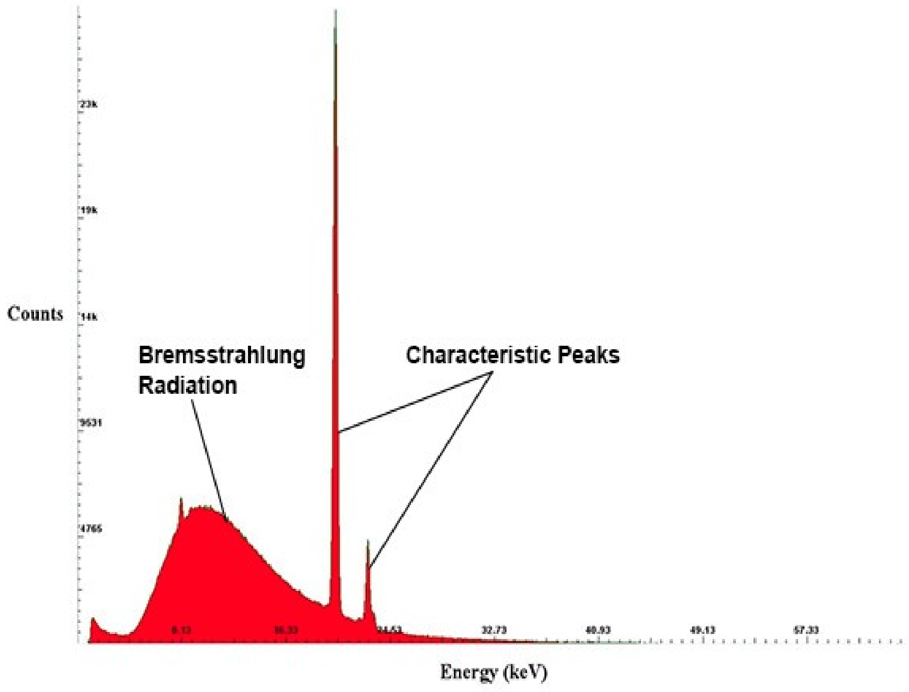
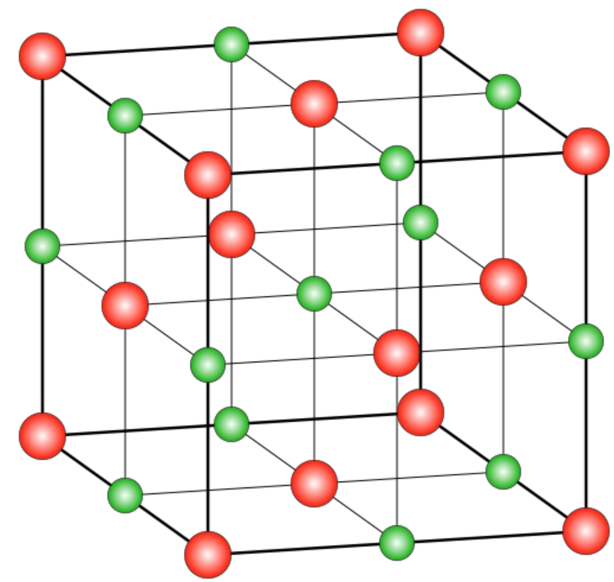
X-Rays

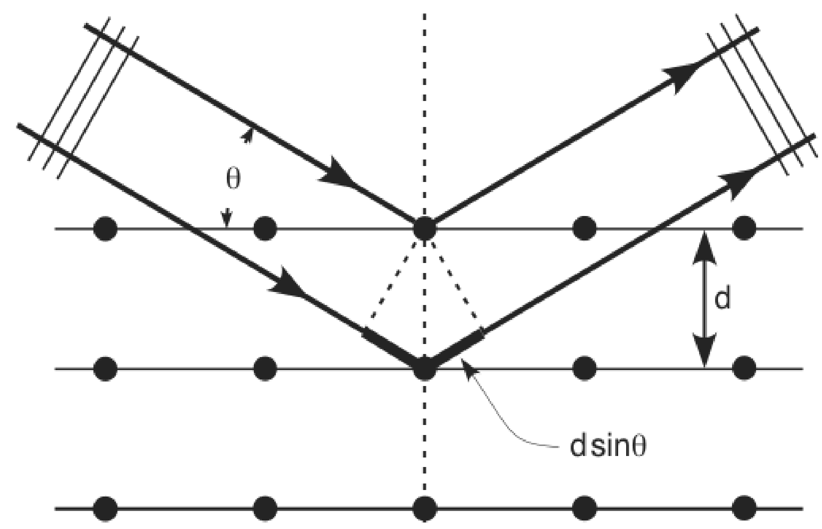
- High-energy EM waves produced by bombarding a target with electrons
- Produced by two principal mechanisms, bremsstrahlung, or braking radiation, and characteristic emission.
- Bremsstrahlung
  - Electrons are decelerated by the electric fields produced in the target; this deceleration leads to radiation
  - Also referred to as 'continuum radiation'
  - Maximum wavelength: λ= ch/eV
- Characteristic Emission
  - Electron 'knocked out' of inner shell; higher-energy electron dropping to fill its place releases an X-ray photon
  - Peaks occur at distinct wavelengths that depend on target material composition



Bragg Diffraction

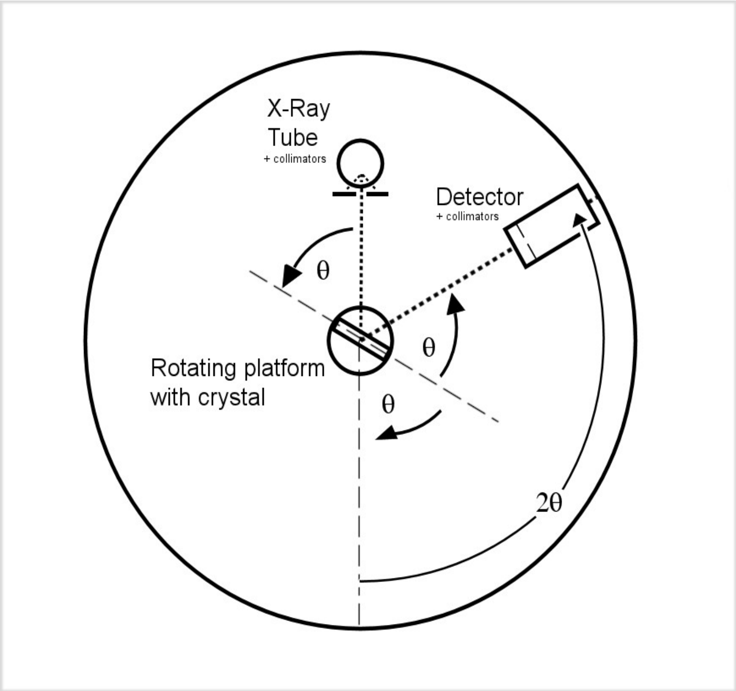
- X-ray wavelength ~1Å
- Spacing between most atoms in crystals is a few Å, so we can treat the crystals as a diffraction grating for X-rays
- Bragg's Law: $2d\sin(\theta)=n\lambda$
- Thus, using X-rays of known wavelength allows us to determine the atomic spacing, and thus the composition, of many crystals





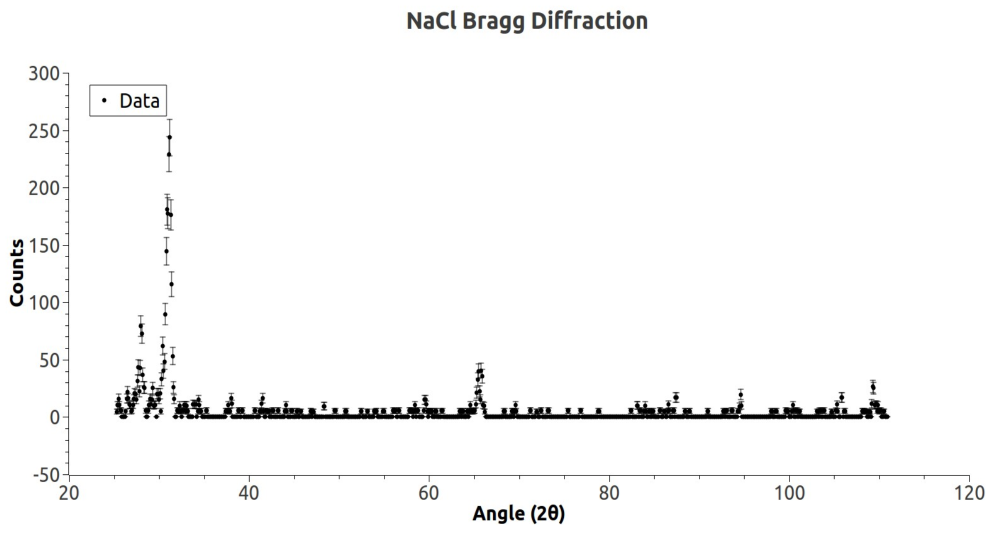
The Tel-X-Ometer

- Consists of a copper X-ray tube, a crystal post, a driving motor, a lead-glass shield, and a Geiger-Müller tube
- Geiger-Müller tube filled with inert gas at high-voltage. Incident X-rays ionize gas molecules, which fly towards the cathode/anode and ionize more particles, creating an 'avalanche'
- X-ray angles of incidence and reflection must be equal, so the driving motor respects a θ-2θ orientation



Bragg Diffraction: Calibration

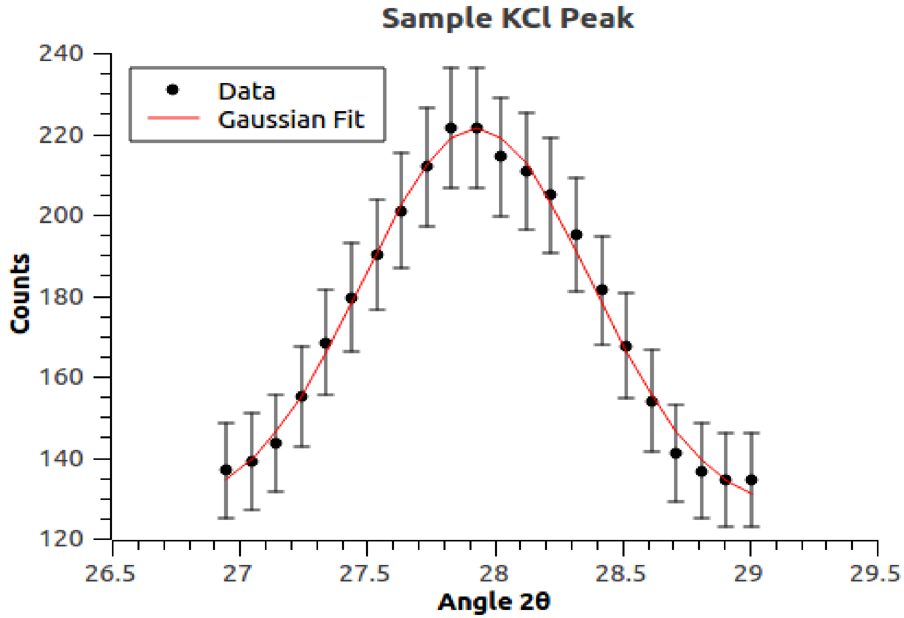
- Calculate NaCl bond length: $d = \sqrt[3]{\frac{M}{2\rho N}} = 0.282\,nm$
- Perform Bragg Diffraction and observe diffraction maxima. Fit peaks to Gaussian distributions.
- Use these results to find characteristic emission peaks of copper (K_α, K_β)



2θ	θ	sin(θ)	Nλ (nm)	λ (nm)
27.569 ± 0.608	13.784 ± 0.304	0.238 ± 0.295	0.134 ± 0.166	0.134 ± 0.166
30.992 ± 0.010	15.496 ± 0.005	0.267 ± 0.005	0.151 ± 0.003	0.151 ± 0.003
57.952 ± 0.059	28.976 ± 0.030	0.484 ± 0.026	0.273 ± 0.015	0.137 ± 0.008
65.087 ± 0.098	32.544 ± 0.049	0.538 ± 0.041	0.303 ± 0.023	0.152 ± 0.012
109.220 ± 0.020	54.610 ± 0.010	0.815 ± 0.006	0.460 ± 0.003	0.153 ± 0.001

Bragg Diffraction: Known Crystals

- Assume K_α, K_β are known:
  - K_α=0.154 nm
  - K_β=0.138 nm
- Perform Bragg Diffraction for known crystals; calculate atomic spacing
- Experiment:
  - LiF: d= 0.202 ± 0.063 nm
  - KCl: d= 0.316 ± 0.158 nm
- Theory:
  - LiF: d= 0.201 nm
  - KCl: d= 0.315 nm



Bragg Diffraction: Unknown Crystal

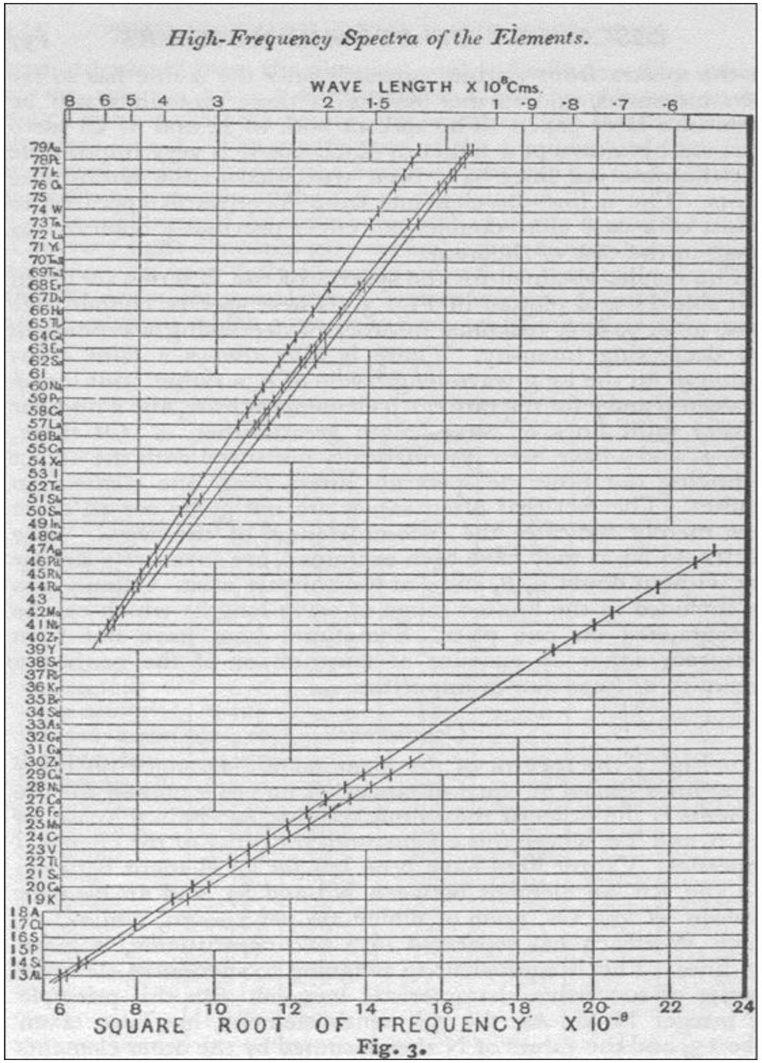
- As before, assume K_α, K_β are known:
  - K_α=0.154 nm
  - K_β=0.138 nm
- Performed Bragg Diffraction for unknown crystal; calculated atomic spacing.
- Measured spacing: d= 0.321±0.100 nm
- Crystal is thus likely KBr, but this is inconclusive

Moseley's Law

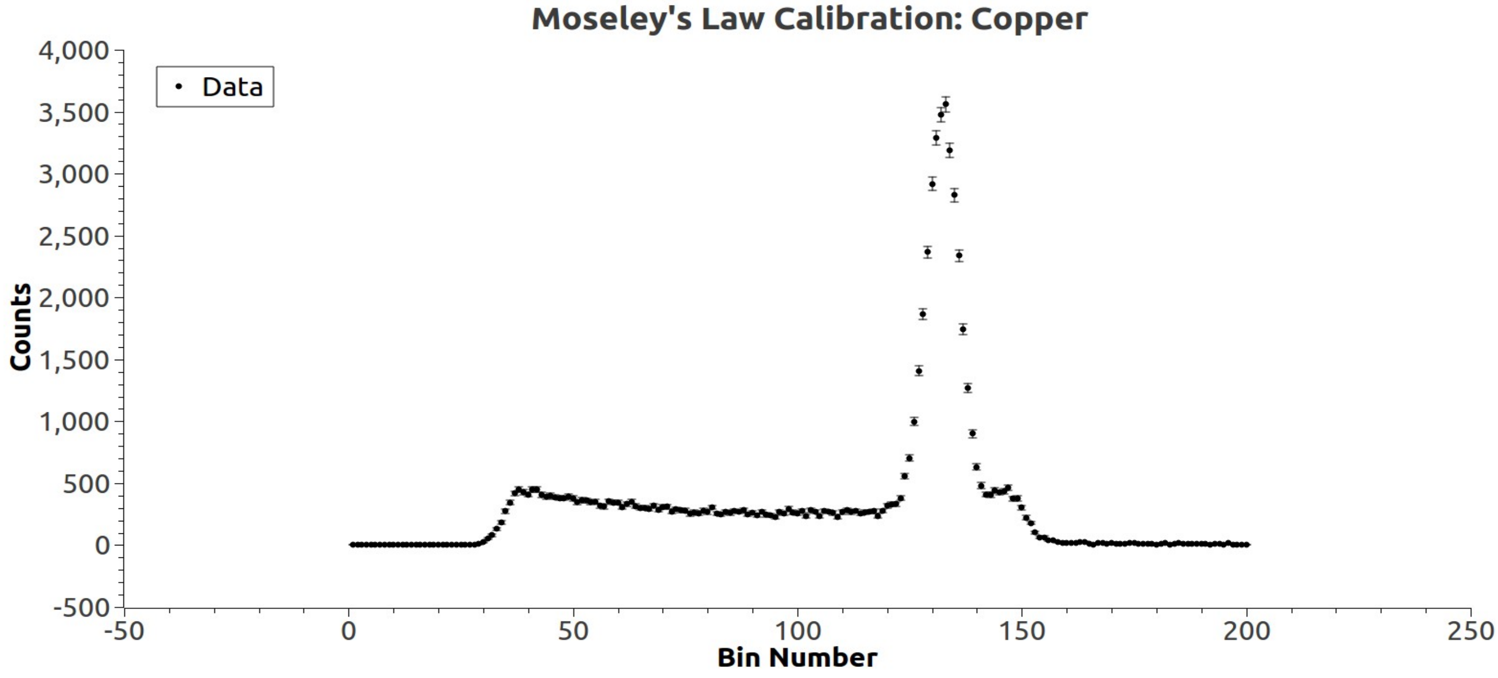
- Characteristic X-Rays for different substances depend on atomic number.
- Bohr Model:

$$E = h\nu = E_i - E_f = \frac{m_e q_e^2 q_Z^2}{8h^2\varepsilon_0^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

- Moseley plotted √f vs. (Z-1) for various metals; we wish to construct a plot of √E vs. (Z-1) for various metals.
- Shows significance of atomic number Z as a physical property

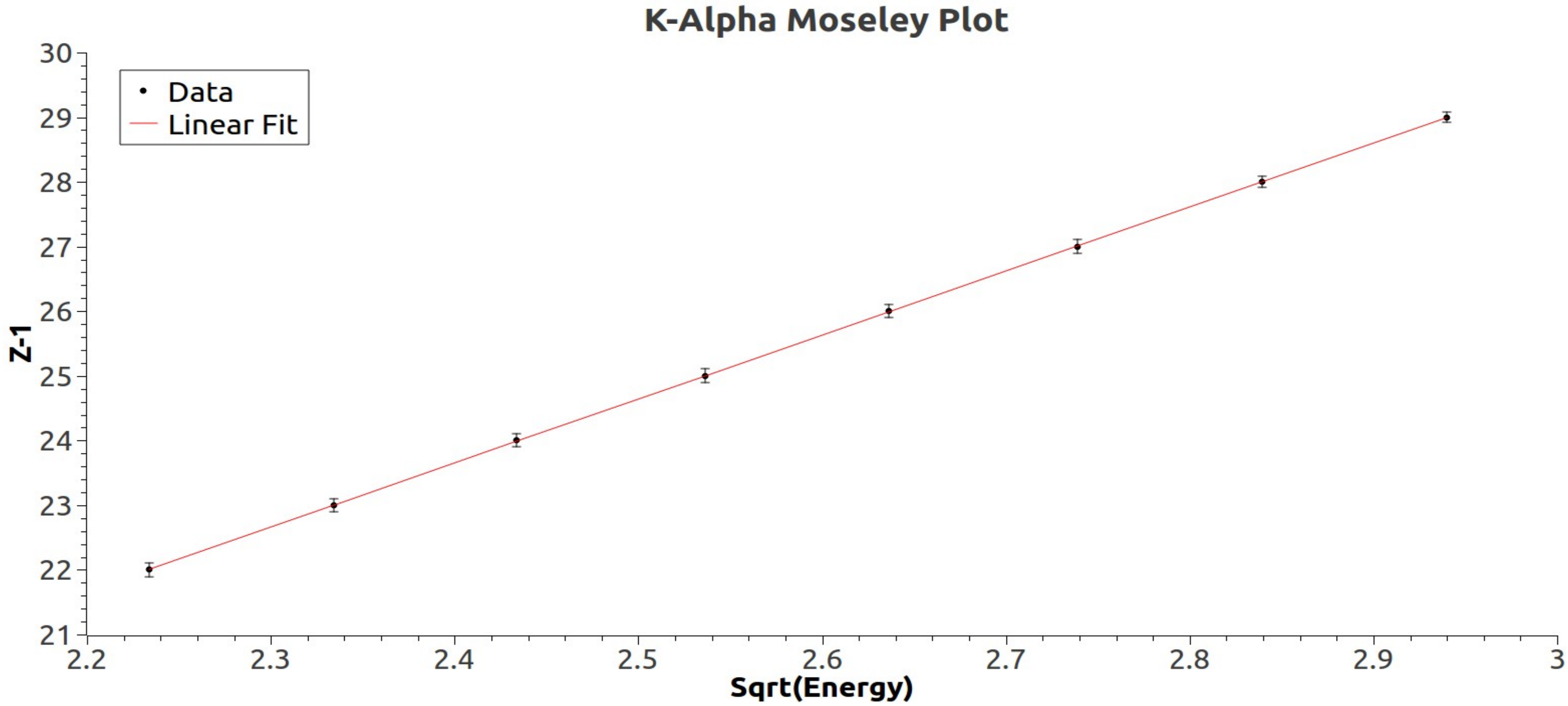


Moseley's Law: Calibration



- Replace GM tube with a silicon PIN diode; fix position of arm
- We use two samples with known K_α peaks to determine energy per bin (Copper and Molybdenum)
- Errors are ~√n because counts follow a Poisson distribution

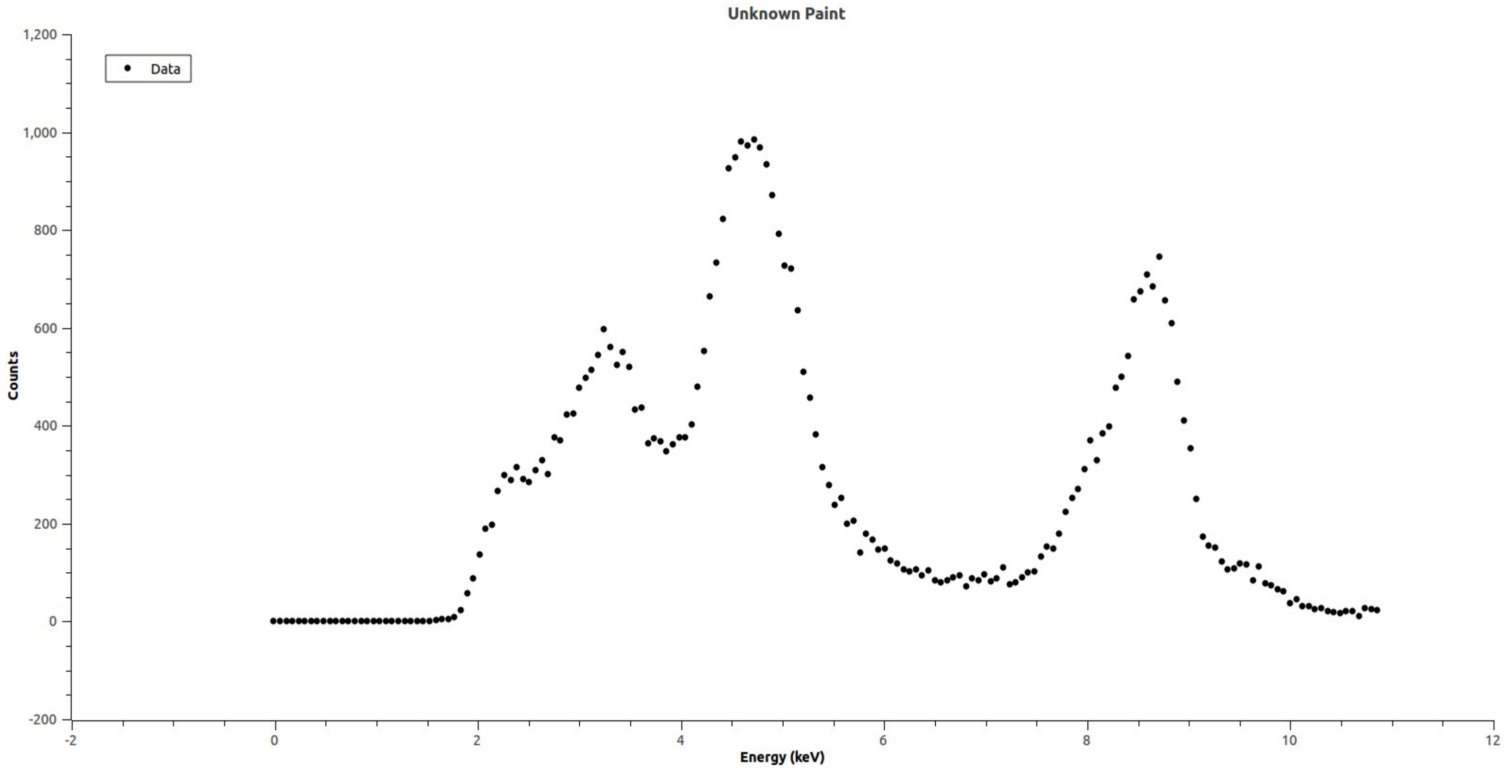
Moseley's Law: Moseley Plot



- We measure K_α values for several metals and use these measurements to generate a plot of K_α energy versus atomic number. Measurements and uncertainties are Gaussian fits
- We can then use this plot to determine the atomic number of unknown samples
- Fit: y= Ax+B, B = -0.112 +/- 0.390, A = 9.902 +/- 0.148
- Chi^2/doF = 0.008
- R^2 = 0.99999

Moseley's Law: Unknown Samples

- The peaks of several unknown samples were correlated with the atomic numbers of their components using Moseley's Law
- Yellow paint: Cadmium, Zinc
- Unknown Metal: Nickel
- Steel 1: Iron, Carbon
- Steel 2: Iron, Carbon, Chromium



Conclusions

- X-Ray Spectroscopy is a useful tool for identifying properties of unknown samples
- Bragg Diffraction allows for identification of crystals based on atomic spacing; if a crystal is known, we can also use Bragg diffraction to identify the characteristic emission spectrum of the source
- Moseley's Law allows for identification of samples' atomic numbers based on their characteristic emission spectra
- By demonstrating the importance of Z, Moseley's Law helped define the periodic table as we know it today

Sources for Figures

- [1] http://www.oxford-instruments.com/businesses/industrial-products/oxford-instruments-x-ray-technology/application-notes/typical-x-ray-spectra-by-anode-material
- [2] https://commons.wikimedia.org/wiki/File:Bragg_diffraction.png
- [3] http://www.graylark.com/eve/lattices.html
- [4] Farrell, Margie. Adapted from Physics 5700 Material, OSU
- [5] Farrell, Margie. Adapted from Physics 5700 Material, OSU