

Lab 4: X-Ray Studies

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1 X-Ray Emission Spectrum

To start the X-Ray analysis, we study the energy-resolved copper X-Ray emission spectrum collected using Bragg scattering.

1.1 Data Handling

We use Bragg scattering to take narrow bins in energy of the spectrum observed. Instead of taking a look at a spectrum of energies, we observe scattered beams that satisfy Bragg's Scattering. The equation governing Bragg's Scattering is

$$n\lambda = 2d\sin(\theta) \quad (1)$$

In this experiment, we assume that the only observed energy is the one satisfying the equation with the lowest order number, $n=1$. This value should dominate the spectrum. The d in the equation represents the distance between neighboring planes of atoms in the crystal, λ is the wavelength of the scattered x-ray beam, and θ is the angle between the incident x-rays and the surface of the crystal. We can set the angle to find wavelength, and the d for all experiments is 0.20 nano-meters. For each angle, and subsequently for each wavelength, we will be measuring the intensity of the X-Ray beam, or the count rate. Then, we can plot the count rate as a function of wavelength to visualize the K_α and K_β energy lines. These lines define the energy needed for an electron to drop from the electron shell $n=2$ to $n=1$ and from $n=3$ to $n=1$ respectively. From there, we can also calculate the Planck constant as a function of the wavelength cutoff. Neglecting the small Bremsstrahlung radiation at high energy, electron high energy cutoff can be related to an x-ray short wavelength cut-off by the equation

$$E = \frac{hc}{\lambda} \quad (2)$$

While taking measurements, we set the current to 10 A with an accelerating voltage of 20 keV.

1.2 Data

We plot the copper X-Ray emission spectrum with a couple of identifying features.

1.3 Analysis

Looking at the spectrum, there are a couple identifiable features. There is a cutoff in the low wavelength/high energy that starts dipping between 0.75 and 1.00 Angstroms. There is another high wavelength/low energy cutoff that asymptotes off after about 1.50 Angstroms, in which the Bremsstrahlung radiation dominates. More noticeably, there are two distinct peaks at around 1.30 Angstroms and 1.45 Angstroms. The lower wavelength/higher energy peak corresponds to the K_β energy peak, while the lower energy peak corresponds to the K_α energy peak. This is known from the fact that it requires

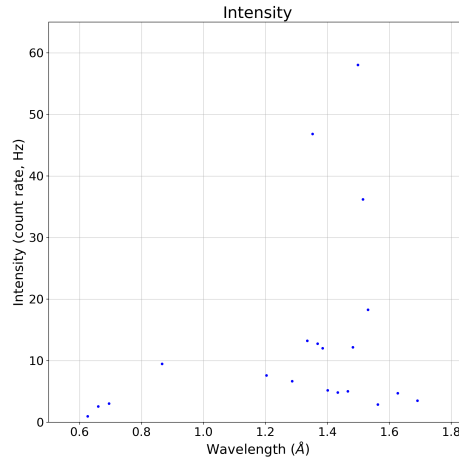


Figure 1: Copper X-Ray Emission Spectrum

more energy to have an electron jump from the third to first energy level rather than from the second to the first energy level.

Looking at the plot, each peak has the two highest amounts of intensity. Indexing into these data points and finding the relevant wavelength, we find fits for the K_α and K_β falling within error of the literature value.

	K_α (Å)	K_β (Å)	h ($10^{-15} eV/Hz$)
Calculated	1.50 ± 0.15	1.35 ± 0.17	4.01 ± 0.04
Literature	1.54	1.39	4.12

Table 1: K lines

To find the high energy cutoff in order to estimate Planck's constant, I created a linear fit to the four data points at the lowest wavelength, and found where the count rate is zero. While taking measurements, we expected a plateauing plot from 0.80Å to 1.25Å. To save time, we did not take many values between there. With only four points at the lower wavelength, the best way to find where the cutoff is zero count rate, would be to simply put on a linear fit. We had to balance saving time to work on other parts of the experiment while also gathering data needed at these lower wavelengths. Measuring more count rates at these lower wavelengths would also be tedious as we would have to wait longer to gather a reliably statistical value, and we may be susceptible to noise. In effect, we simply made a linear fit and found where the intensity was zero for the high energy cutoff and estimated Planck's constant using equation 1.

The calculated Planck's constant does not fall within error bars of the literature value.

1.4 Uncertainty

The count rate is just calculated as a count divided by time. Since we used software to stop the time, we assume that the uncertainty in time is negligible as any uncertainty between us clicking stop on the timer to the software to communicate within itself must be very very small. In effect, the only uncertainty in the count rate would be in the count, which is just the error in a Poisson distribution

$$dC = \frac{1}{\sqrt{C}} \quad (3)$$

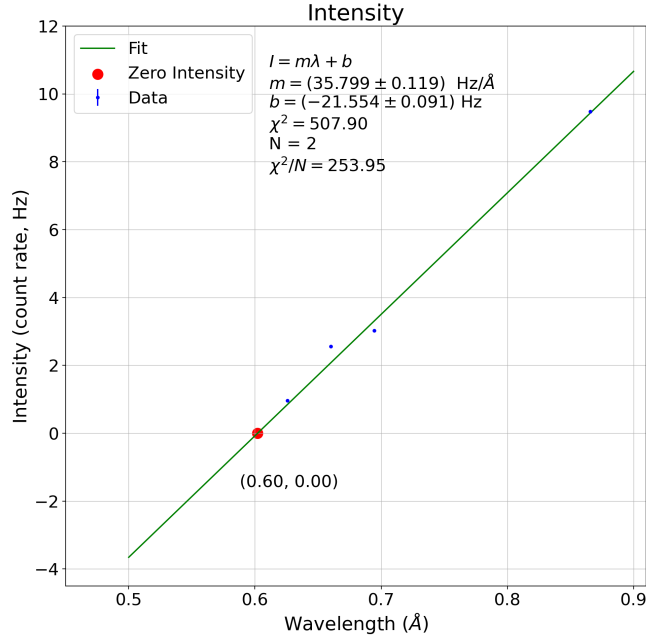


Figure 2: Low Wavelength Linear Fit

where C is the net count rate. When calculating the specific wavelength at which the K_α and K_β values are at, there is some uncertainty in this wavelength. To calculate this uncertainty in a spectrum's peak, I multiplied the uncertainty in this "peaky" value by the uncertainty in the placement of the peak. The uncertainty in the peaky value would be simply the Poisson error of the count rate, which is the same as equation 3. The uncertainty in the placement of the peak is 1 standard deviation in the spectrum's peak. To calculate this, we divided the Full Width Half Max by 2.42. In effect the uncertainty in a wavelength would be

$$d\lambda = \frac{FWHM/2.42}{\sqrt{C}} \quad (4)$$

To calculate the uncertainty in Planck's constant, I used the usual uncertainty of a function

$$\Delta f = \sqrt{\left(\frac{\partial f}{\partial x_i} \Delta x_i\right)^2 + \left(\frac{\partial f}{\partial x_{i+1}} \Delta x_{i+1}\right)^2 + \dots} \quad (5)$$

In this case, the only input for to calculate Planck's constant is the wavelength, so

$$dh = h d\lambda \quad (6)$$

Despite using these error analysis tools, I believe there is room to improve in the error analysis for four reasons. The first is that just looking at the spectrum, the data looks like scatter points, when the error bars should be more pronounced. Furthermore, the linear fit seen in the second figure has a very high reduced chi square despite the fit seeming to follow quite well. This indicates that the error bars are too small and not all errors may be accounted for. Next, the measurements near the low wavelength will have lower count rates. When taking more and more points near the energy cutoff, we will only be receiving a small amount of intensity, and anything past the high energy cutoff will most likely be noise. This noise can make calibrating the linear fit for Planck constant have lots of uncertainties, but it is hard to quantify without taking more data and fitting a higher order polynomial. Finally, to

accurately propagate an uncertainty in the wavelength, we would have to account for the uncertainty in the angle set and measured.

2 Moseley's Law

The next study is dealing with finding a relationship between atomic number and the K line energy for different elements. We want to investigate Moseley's Law.

2.1 Data Handling

Instead of using Bragg scattering, we measured using only the energy resolution of the proportional counter. We no longer specifically look at copper's x-ray emission and absorption spectrum.

We first used the extremities of our elements available, Vanadium ($Z=23$) and Zinc ($Z=30$) to calibrate our spectrum to measure for energies. The PHA spectrum software in the lab computer allows us to do this. When measuring the count rates, we had the metal foils striking straight onto the photomultiplier tube at a 90 degree angle. Afterwards, we set the tube voltage to 29.7 keV and the beam current to 10 Amps to start measuring count rates. After calibrating, we observed the spectrum to find a peak that would encompass the K lines.

Then we fit the data to a linear fit to investigate Moseley's law of

$$E = 0.75hcR(Z - 1)^2 \quad (7)$$

This implies that $(Z - 1)^2$ is linearly related to the K energy by the slope of $0.75hcR$, where h is Planck's constant, c is the speed of light, and R is the Rydberg constant.

2.2 Data

Here is our data and linear fit to the K line compared with the atomic number.

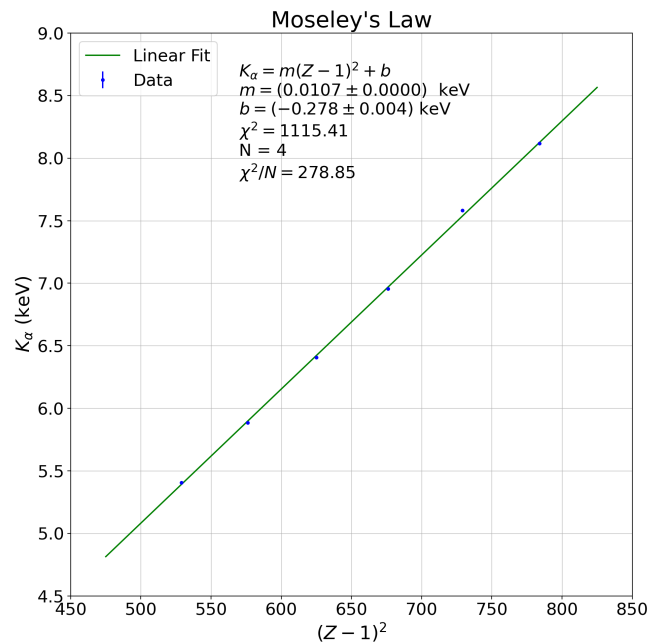


Figure 3: Moseley's Law with Linear Fit

The K line was found for Iron, Cobalt, Nickel, Chromium, Manganese, and Copper.

2.3 Analysis

Using these energy values, we can compare the Rydberg energy ($E_R = hcR$) to see how well our data fits to the literature value. For this, we have to multiply the slope of the linear fit by 4/3, as can be seen from some simple algebra.

$$E = 0.75hcR(Z - 1)^2$$

$$y = mx + b \rightarrow x = (Z - 1)^2$$

$$m = 0.75hcR = \frac{3hcR}{4} \rightarrow E_R = hcR = m \frac{4}{3}$$

	E_R (eV)
Calculated	14.29 ± 0.01
Literature	13.61

Table 2: E_R values

The calculated Rydberg energy is out of error bars, but it is within an order of magnitude, just being off by one electronvolt. Despite not having our Rydberg energy within error bars, the general linear fit of the plot is strong.

2.4 Uncertainty

To calculate the K line, I used the centroid, or weighted average, for a measurement's spectrum peak. The uncertainty in this centroid energy is similarly calculated as wavelength uncertainty in the last experiment, described by equation 4. From this, the uncertainty for the graph of K line, is known.

The uncertainty in the Rydberg energy comes from the linear fit's error. Then multiplying by the appropriate constants to get an uncertainty in the energy, E_R , which is what's in Table 2.3. Similarly as equation 6

$$dE_R = R_E m \tag{8}$$

where m is the slope for the linear fit.

An interesting feature from the linear fit is the rather high reduced chi squared value. Looking at the graph, the green linear fit does correlate with the data very well, so this implies that the error of the K line may not be properly accounted for in this experiment.

3 X-Ray Absorption Spectrum

The third and final study is dealing with finding a relationship between high energy absorption cutoff and atomic number. To complete this, we use Bragg's Scattering.

3.1 Data Handling

Similarly to the first experiment, we will measure the count rate intensity for a specific angle. But we are not necessarily interested in just a raw intensity, we would like to find the proportion that a metal foil will absorb a copper x-ray emission. In effect, we have to calculate both the count rate with the metal foil and the count rate without any foil - this provides the fraction that is absorbed by the foil. Afterwards, we would like to measure this proportion at different angles, to help find the high energy

absorption cutoff. Further, to find a relationship with the atomic number, we need to complete these measurements for different elements. Then, we can compute the high energy absorption and compare to the literature value of the binding energy for that element. We should see something similar to Moseley's law, in which the higher the atomic number, the higher energy. However, we used the K lines emission spectrum for that, and here we will use the absorption cutoff.

3.2 Data

When completing this experiment, we ran short on time and weren't able to clearly resolve absorption edges for all elements. Here is the relative absorption for Copper, Nickel, and Cobalt.

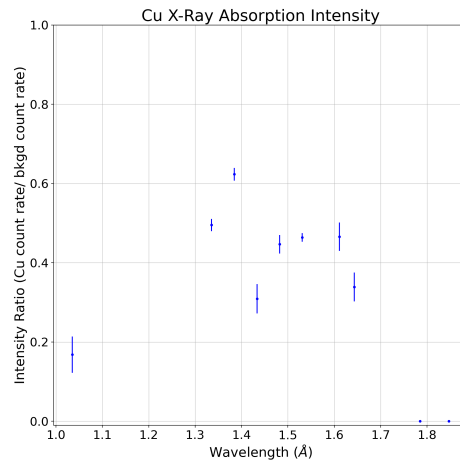


Figure 4: Relative Copper X-Ray Absorption Spectrum

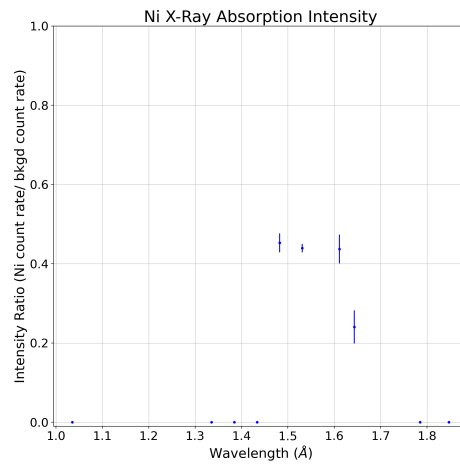


Figure 5: Relative Nickel X-Ray Absorption Spectrum

Here, we can see that the absorption edge for Copper should be below 1.00 Angstroms, for Nickel it should be near 1.45 Angstroms, and for Cobalt it should be around 1.55 Angstroms. In this study, we estimate the cutoff to be the midpoint between the lowest wavelength with non-zero intensity and the highest wavelength with zero intensity. We use this to account for the low resolution in the ratios

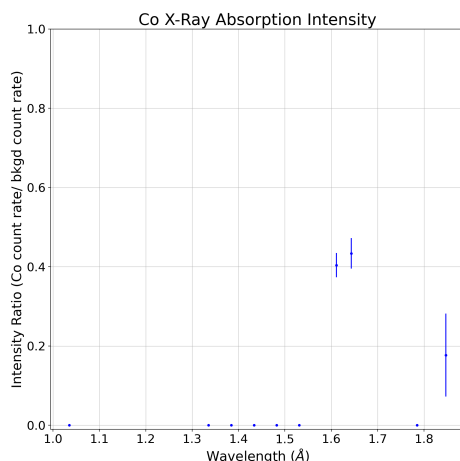


Figure 6: Relative Cobalt X-Ray Absorption Spectrum

calculated. Without much more data, we can't specify a wavelength where the intensity starts being 0, so we use this midpoint as an estimate for where it should be 0. For Copper, we did not measure an intensity with zero at high energy, so we estimate the absorption cutoff simply as the lowest wavelength, as we cannot make any assumption or data fitting outside of our domain.

3.3 Analysis

To calculate the high absorption energy, we use the relationship between wavelength and energy, as seen from equation 2. Then we can compare with the literature value for each absorption edge's energy.

Element	Wavelength (\AA)	Calculated E (eV)	Literature E (eV)
Cu	1.04 ± 0.05	11.63 ± 0.53	8.98
Ni	1.43 ± 0.02	8.40 ± 0.20	8.33
Co	1.55 ± 0.03	7.79 ± 0.24	7.71

Table 3: High Energy Absorption Values

Despite the calculated energy cutoff not being within error of the literature value for Copper, the other elements are within the high energy cutoff literature value. The general trend with respect to atomic number is the same as Moseley's Law: the larger the atomic number, the higher the energy. In effect, we would expect larger atomic numbers to present a lower wavelength cutoff. From the following plot, we can see that this is actually the case. The lowest cutoff is Cu, then Ni, then Co, which correlate with atomic numbers.

However, just looking at figure 7 shows that it is not displaying the full picture. A lot of the ratios that are at zero were only measured for 30 seconds before we decided that this will just produce a negligible count rate. With more time, we could leave these measurements going for longer, and take measurements at many more angles. This would better resolve the high energy cutoff.

3.4 Uncertainty

The uncertainty for the count ratio is defined by the uncertainty in the counts measured, so this is the Poisson error, as equation 3 describes. These uncertainty values are the uncertainty bars shown in figures 4, 5, 6, 7. To calculate the uncertainty in energy, we use equation 4, which describes the peak where we set our region of interest and the distribution of that peak, using 1 sigma and the counts. As

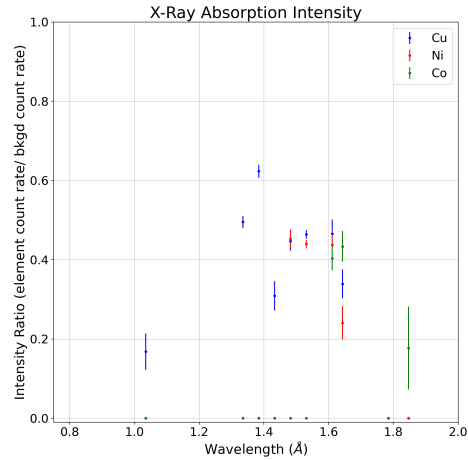


Figure 7: Relative X-Ray Absorption Spectrum

mentioned before, this is not perfect and does not account for all uncertainties, as can be seen from how well our data matches the literature values.

4 Conclusion

Three X-Ray studies were conducted to investigate copper x-ray emission spectrum, Moseley's Law, and the x-ray absorption spectrum for different elements. From the first experiment, our data does not fall within uncertainty of the K lines to properly conclude anything. Likewise, the Planck's constant calculated was not within error bars. Despite finding these values within an order of magnitude of the literature values, our findings are inconclusive. For the Moseley's Law experiment, we found a very well fitted linear relationship, but the calculated Rydberg energy fell outside the literature value. With this, we can conclude that our relationship, despite being linear, does not conclude Moseley's Law. Finally for the third experiment concerning the absorption emission spectrum, we found our energy absorption not within uncertainty values with the literature binding energies for those elements. In effect, we cannot conclude much from our experiment, but the general trend can be seen such that the larger the atomic number, the higher the energy spectrum. The uncertainties throughout the studies were explained in each section, but can be improved upon.