X-Ray Studies

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Abstract

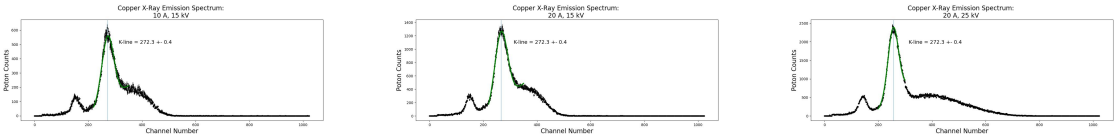
X-ray fluorescence spectra that are used to characterize elements consist of two main features: discrete characteristic radiation peaks and a continuous bremsstrahlung spectrum. This report studies both characteristic radiation and bremsstrahlung radiation using two different methods of observing x-rays: a proportional counter and Bragg's scattering. In the first section, I experimentally test Moseley law relating the K-alpha characteristic radiation peak and atomic number by observing the characteristic radiation peaks of various elements using the method of the proportional counter. In the second section, I create a full spectrum for copper using the method of Bragg's scattering.

Introduction

X-rays are electromagnetic waves that occupy energies in the range of 0.1 to 100 keV. When x-rays hit a target material, two types of x-rays can be observed: characteristic radiation or bremsstrahlung radiation. Characteristic radiation is the phenomenon in which an x-ray emits secondary x-rays, known as x-ray fluorescence, upon knocking out the inner-most electron shell of the target material. Specifically, it is characteristic of an element because the energy required to overcome the binding energy of the k-shell is dependent upon atomic number. In contrast to characteristic radiation that comes in peaks at discrete energies, bremssttrahlung radiation is emitted in a continuous spectrum because of the attractive force between the negatively charged accelerated electron and the positively charged nucleus that alters the trajectory of the electron, thereby slowing it down accompanied by a loss of kinetic energy. Crucially, the electron cannot give off more energy than it has, which creates a high-energy cutoff. This high-energy cutoff is directly proportional to the accelerating voltage (Fig. 1). These three features of the characteristic radiation peaks, the brehmsstralang spectrum, and the high-energy cut-off form the full-energy spectrum for a unique element.

Methods

Our set-up consisted of a Tel-X-Ometer that produced the x-rays by accelerating electrons in the x-ray tube. The x-rays can be detected via the proportional counter as well as Bragg's scattering. The proportional counter utilizes the cascading effect of ionizing electrons in a voltage of +2100 Volts. Because each electron undergoes secondary ionization, the pulse of detected electrons that strike the anode is proportional the incident x-ray energy. However, using this method, we were unable to distinguish between the K-alpha and K-beta peaks because of resolution limitations of the proportional counter. In order to achieve higher resolution, we used the second method: Bragg's scattering. In Bragg's Scattering, we indirectly detected x-ray energies by way of diffracting the incident x-ray beam through a lithium crystal lattice at various angles. The intensity observed is the result of constructive interference when wavelengths of x-rays are in phase according to the Bragg's scattering equation: $n\Lambda = 2dsin\theta$. Using this equation, we were able to convert the angle of diffraction into wavelength, or energy, giving the indirect observance of x-ray energy and intensity.



(a) (b) (c)

Figure 1: Direct copper full-emission spectra at different accelerating voltages and intensities. The location of the characteristic radiation peak remains the same under all parameters, while the bremsstrahlung cutoff increases under the higher accelerting voltage of figure c and the photon count increases under the higher current in figure b. The calibration settings- coarse gain: 4, fine gain: 0.

1 Testing Mosley's Law

After calibrating for the energy (Fig.2), we directly measured the energy of the characteristic line for seven different elements with z-values between 23-30: Vanadium (23), Chromium (24), Manganese (25), Iron (26), Nickel (28), Copper (29), Zinc (30), using the proportional counter (Fig. 3). The uncertainty in the energy was calculated by fitting a Gaussian function with linear background to the characteristic peak for each of the seven elements. The uncertainty of the energy was then calculated to be (the uncertainty in the fitted peak $\times$ 31.48) + 15.07, using the calibration of channel to energy. This propagation does not take into account the uncertainty in the calibration parameters.
Due to resolution limitations of the proportional counter, we were unable to distinguish between the k-alpha and the k-beta peaks such that the recorded channel value and corresponding energy was higher for every element than as predicted by Mosely's law that predicts only the K-alpha peak, and specifically does not include the k-beta (Figure 5). In order to test this hypothesis that the resolution limitation caused over-estimation of the energy, the average of literature values for K-alpha and K-beta for each element is also plotted.[1] The observed data was statistically more similar to the averaged peaks in literature than to Mosely's law shown by the residuals more randomized around zero (Figure 4). This shows that our observed energies for each element over-estimated the predicted energies as modeled by Mosely's law due to our including of the K-beta peak. Although our observed energies differed in terms of magnitude with Mosely's law, the relationship was correlated as the slope of the Mosely's law model is within 2.5 error bars of the slope of the observed.

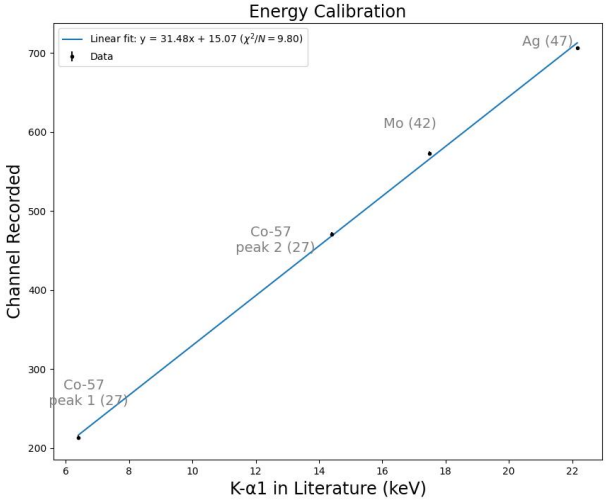


Figure 2: The calibration plot relating the channels of observed peak and literature value peaks for Co-57, Mo, and Ag. Line of best fit parameters are m: 31.48 $\pm$ 0.21 and b: 15.07 $\pm$ 3.5 Calibration settings- coarse gain: 4, fine gain: 0.

[1] $https://xdb.lbl.gov/Section1/Table_1 - 2.pdf$

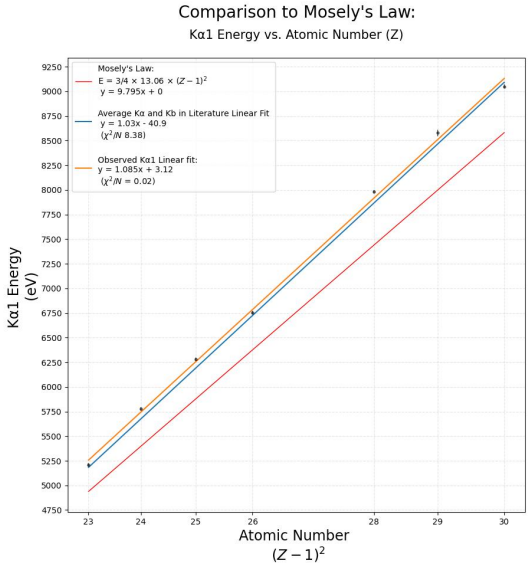
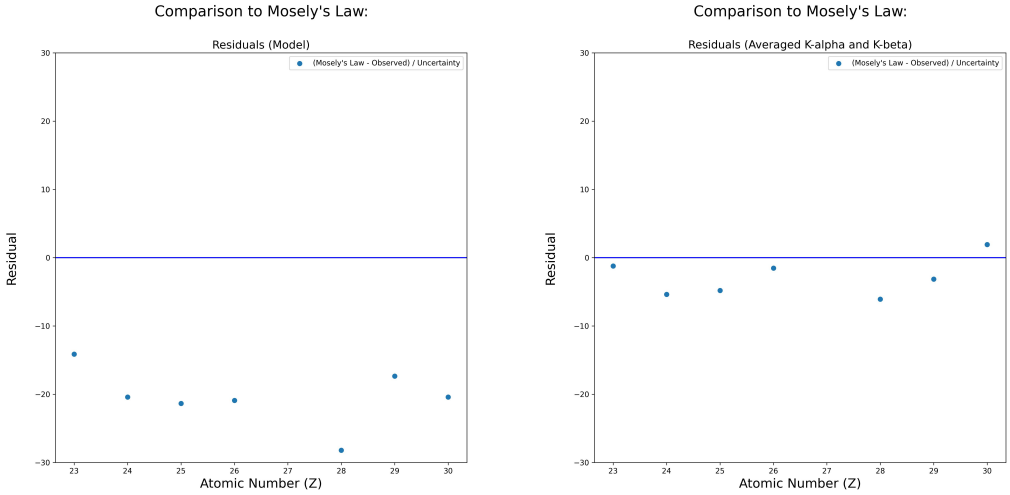
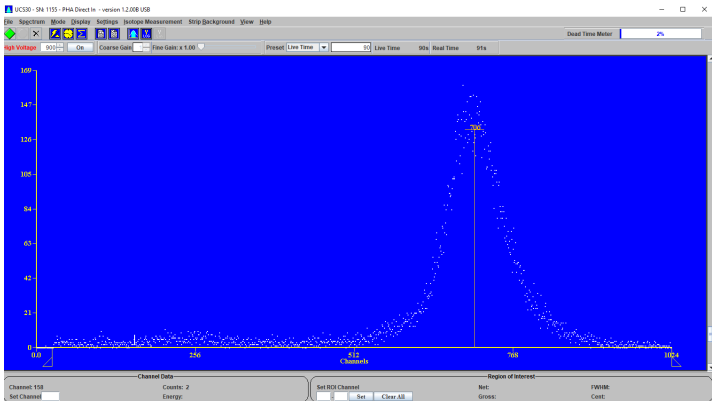


Figure 3: Observed energies, predicted energies by Mosely's law, and averaged energies in literature by atomic number. Note that while the energies differ in terms of magnitude between the observed values and Mosely's law, the correlation is similar as evident by their slopes. Higher correlation is seen between the observed values and the averaged literature values.

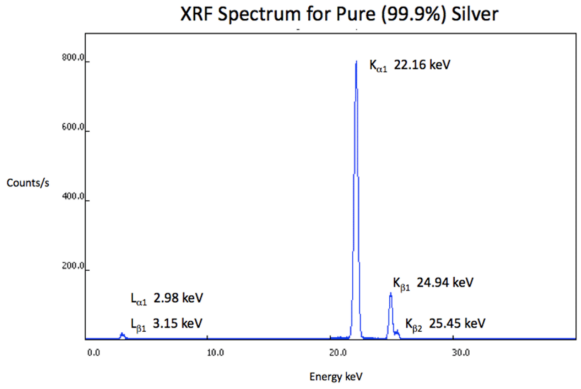


(a) (b)

Figure 4: Residual plots for observed data compared to Mosely's law (a) and observed data compared to the averaged literature values for K-alpha and K-beta peaks (b). Note that the residuals with respect to Mosley's law are all greater in magnitude than the residuals with respect to the averaged peak values in literature, indicating more similarity in the latter.



(a)



(b)

Figure 5: The direct spectrum for Ag as detected by the proportional counter (a) and the spectrum for pure silver from literature.Note that the K-alpha and the K-beta peaks of the spectrum from literature are indistinguishable on the direct spectrum we observed. [3]

2 Full Spectrum

The full x-ray emission spectrum for copper was obtained through Bragg's scattering. Specifically, we detected the count of x-rays hitting the detector at different diffraction angles by rotating the detector. Because the characteristic radiation peaks are discrete, incrementally rotating the detector from 0 degrees to 90 degrees may have caused us to miss the peak, while also causing us more time by acquiring extraneous data points for the brehmsstralang radiation that are not characteristic to the element. In order to ensure that we detected the peaks and optimized for the number of data points acquired, we first turned on the rate meter audio and rotated the detector; loud noises indicated higher rates which we could identify as a peak and a softer noises indicated the high-energy cutoff where the rates fell off. This gave us preliminary knowledge of which angles required the most data points: k-alpha at the 45 degree angle, k-beta at the 40 degree angle, and the high-energy cut-off at the 28 degree angle.

We started at angle 39.67 and moved in increments of .17 degrees through angle 40 until angle 41.33. We knew to stop at 41.33 because we were roughly plotting the data as we collected, and at 41.33, the peak was complete.For the second peak, we used a different method, that contributed to more error. Instead of sweeping continuously through the angle in one direction, we started at 45 degrees and detected in increments of .17 degrees to 45.5 and then went in the opposite direction, detecting in increments of -.17 degrees to 44.33. Switching directions invites error due to backlash of the gear. For the brehmsstralang radiation, we collected data in one direction in various increments. Angles were chosen by looking at the rough data we were plotting and identifying where data points would be necessary to discern the shape of the brehmsstralang spectrum. We detected the high-energy cut off while doing so.

After collecting the counts at each angle, I fit the counts at every angle to a Gaussian function that gave the area under the Gaussian that gave intensity by dividing by acquiring time, which was 90 seconds for the peak measurements and 30 seconds for the brehmsstralang radiation measurements. Next, the Bragg's scatting equation was used to convert angle into energy for each data point:

$$n\Lambda = 2dsin(\theta) \rightarrow \Lambda = 2(0.208nm)sin(\theta)/2 \rightarrow E = 1240/\Lambda \ .$$

While I collected uncertainties for the intensity with each Gaussian fit, these were negligible compared to the uncertainties in the angle measurement that I chose to focus on. I calculated the uncertainty in the energy due to the angle uncertainty of .17 degrees as follows: (Where 0.17 degrees is the uncertainty in the angle measurement chosen because it is the smallest unit on the angle rotatory; $\cos(\theta)\times$ uncertainty was the uncertainty due to the sin function in Bragg's scattering.)

$$\text{Step 1: } 0.17 \text{ degrees} \rightarrow 0.00289 \text{ rad}$$

$$\text{Step 2: } 0.00289 \times cos(\theta)$$

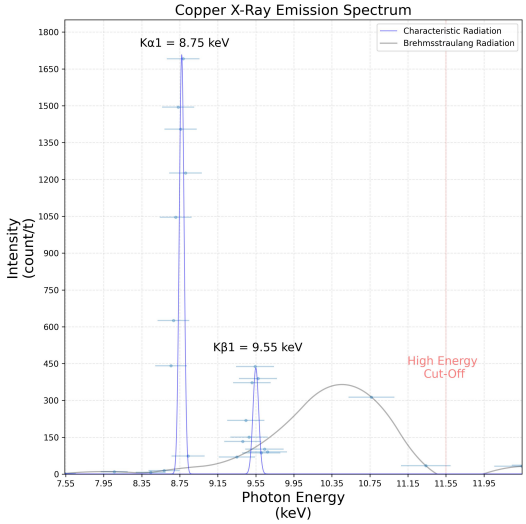
The full spectrum was then plotted as the intensity for each energy with error-bars for the uncertainty in the energy due to the angle uncertainty. (Fig. 6) The K-alpha line was determined as the left peak because K-alpha necessarily has a higher intensity than K-beta because the probability of an electron transitioning from the L shell to the K-shell as happens in the K-alpha peak is greater than the probability of an electron transitioning from the M shell to the K-shell as happens in the K-beta peak. The specific values of each peak took into account both the uncertainty of the energy and the uncertainty in the peak when plotted. The uncertainty was unavailable from a Gaussian fit because the data did not fit. Instead, the uncertainty was determined visually by me as the range of points that constituted the peak, giving the range for the K-alpha peak: [8.68, 8.83] keV and K-beta peak: [9.38, 9.64] keV. The combined uncertainty therefore, was determined to be the range of the left-most bound of the energy of the left-most bound of peak to the right-most bound of energy of the right-most bound of peak. This gave he following:

[3] $https://www.xrfresearch.com/xrf-spectrum-silver/$

	Bragg's Scattering	Proportion Counter	Literature
K-alpha	8.75 +- 0.35	8.4 +- 0.02	8.05
K-beta	9.55 +- 0.375	8.4 +- 0.02	8.91
High Energy Cut-Off	11.55 +- 0.24	14.4 +- 0.01	–

Table 1: Table of the feature energies as observed experimentally using the Bragg's Scattering method, the Proportional counter, and as reported in literature.

Comparing these results to the preliminary direct Copper x-ray emission spectrum yields similarity. The average of the K-alpha and K-beta lines of the Bragg's scattering x-ray emission spectrum is 9.15. Therefore, the direct spectrum that yields the K-alpha and K-beta peak at 8.4 keV is within two error bars of the average of the K-alpha and K-beta peaks of the final spectrum. The high-energy cut-off is within 12 error bars, which is not statistically similar. This dissimilarity is likely due to the voltage not being what we recorded it to be because the High-energy Cut off is necessarily directly proportional to the voltage applied. Comparing these results to the literature values yields similarity. The K-alpha and K-beta peaks are both within 2 error bars of the literature values.



(a)

(b)

Figure 6: The Final Spectrum for Copper using Bragg's Scattering (a) and the Preliminary Spectrum for Copper using the proportional counter (b) Both were observed with settings of 20 uAmps, 15 kV, and a Calibration of coarse gain: 4, fine gain: 0.

Conclusion

Accurately producing the characteristic spectra for elements has applicable importance in x-ray imaging of the body for health reasons as well as having experimental importance in identifying materials used for research reasons. Testing different methods for producing characteristic spectra is important in a lab setting because faulty equipment and methods may yield spectra for materials that align with literature values of the wrong element than what is being used in the experiment. Therefore, this report investigates the performance of two different methods in producing characteristic spectra for Copper that may guide choices about which method of x-ray detection one should use for identifying an element in the lab.

While the first method of the proportional counter over-estimated the energies predicted by Mosely's law because it was not able to resolve between the K-alpha and K-beta peaks, this method nevertheless appeared to do better in determining the K-line energy value of Copper than the method of Bragg's scattering. Specifically, the percent error of the Proportional counter peak of 8.4 and the averaged literature values of 8.48 is less than 1%, while the percent error of the Bragg's scattering K-alpha peak and K-beta peak with literature is 10.5% and 5.8% , respectively. The better performance of the proportional counter method in determining the k-line peak of Copper is likely due to underestimating the uncertainty of both the energy and the intensity in the method of Bragg's scattering. Specifically, my uncertainty did not take into account the variation in counts between channels such that even though there was a negligible uncertainty of the Gaussian-fitted peak, even being one channel off could change the count by between 10 up to 100 counts. While performing this more rigorous uncertainty calculation may improve the shape of the peaks, the bigger problem with was not the shape, but rather, the problem was that the K-alpha and K-beta energies both overestimated the literature values in a way that the the proportional counter method did not. Therefore, more rigorous uncertainty calculation in photon energy would yield more improvement in the peak energies being as predicted by the literature values. Specifically, a more rigorous uncertainty would include the affect of the blacklash due to the gears in the angle rotary. I chose not to include this error, because I did not have a way to quantify it. An experiment could be set-up that tests how the movement of the rotary affects angle observed.

Along with improving upon the Bragg's Scattering method for a more accurate determination of the literature-valued characteristic peaks, the high-energy cut off point can also be further investigated. Specifically, the discrepancy between the high-energy cut-off in the proportional counter and in the Bragg's scattering method is puzzling because high-energy cut-off is directly proportional to the accelerating voltage and both were conducted under the same voltage. This means that a future study can ensure more accurate voltage readings and investigate the result if it reoccurs.

In summary, while the proportional counter over-estimated the Mosely's law energies because of limited resolution, it calculated the characteristic peak for Copper with less error than the Bragg's Scattering method; however, with proper treatment of the energy and angle uncertainties as well as performing the Bragg's Scattering experiment again with more sensitivity to the angle rotary, the method may be improved. If improved in this way, the method of Bragg's Scattering would be more reliable for classifying elements because of having higher resolution than the proportional counter.