Investigating the X-Ray Emission Spectra for Various Materials & Minerals

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Abstract

In this work, we measured the X-ray emission lines of different elements such as molybdenum, copper, nickel, and titanium. Using the known emission energies expected for each element, we were then able to calibrate our system. Using this calibration, we were then able to determine the elemental composition of an unknown source, a 10 cent Israeli shekel coin, and the minerals Strontianit and Pyrrhotin.

Contents

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1 Introduction

1.1 Experimental Setup

As seen in Figure (1), the experimental setup for this work relied on an X-ray unit consisting of an X-ray tube on the left and a measurement chamber on the right, and a goniometer which was found in the measurement chamber. The detector of the chamber was connected to a multichannel analyzer (MCA), which transmitted output to a computer.

Figure 1: The experimental setup

1.2 Theory of the Experiment

1.2.1 X-Ray Tube Emission

When high energy electrons interact with an atom, the electric field of the atom's nucleus can decelerate the electron and cause the emission of a continuous spectrum called bremsstrahlung. This is one type of radiation that is emitted from our X-ray tube.

Another type of radiation can occur when an electron has sufficient energy to ionize a neighbouring atom. In this case, another electron from a higher energy level in the atom will transition to occupy the previous quantum state of the ionized electron, thereby emitting a photon in the process. This photon's energy is correlated to the energy gap between the replacement electron's initial and final energy levels in the atom. This is seen in the following formula:

$$hv_{photon} = E_{initial} - E_{final} \tag{1}$$

where h is Plank's constant, v_{photon} is the photon's frequency and $E_{initial}, E_{final}$ are the initial and final energies of the electron. This type of radiation is known as the characteristic X-ray spectrum. We can use this spectrum to identify the makeup of different alloys and materials.

1.2.2 X-Ray Fluorescence

Another method to generate the characteristic X-ray spectrum is to use X-ray fluorescence. In this method, the material being studied is bombarded by high energy photons. These photons then ionize the materials atoms, causing them to emit the characteristic emission lines. Note that in this method there is no bremsstrahlung being emitted.

2 Results

Each of the following diagrams were obtained by placing different materials in the measurement chamber of the X-ray unit. In the X-ray tube, a beam of accelerated electrons hits the tube's anode, causing the emission of bremsstrahlung radiation and the characteristic X-ray lines of the anode's metal. The X-ray radiation then passes through a small hole into the measurement chamber, from which it proceeds to ionize the material placed there. The emitted spectrum from the material is then measured with the energy detector.

Note that in our case, we used a molybdenum X-ray tube, so for the molybdenum spectrum, no materials were placed in the chamber. Additionally, it is possible that some of the peaks in the spectra obtained in each of the various experiments were actually from the X-ray lines of the molybdenum (and possibly some copper residue) and not from the material placed in the chamber.

2.1 Molybdenum Spectrum

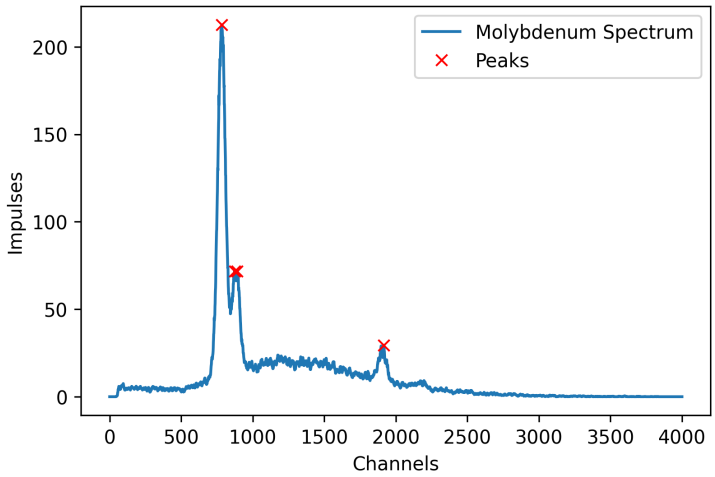

Figure 2: The X-ray emission spectrum of molybdenum

2.2 Copper Spectrum

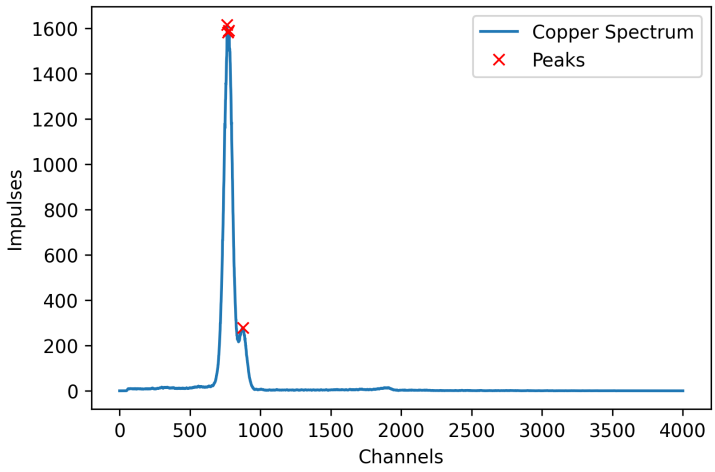

Figure 3: The X-ray emission spectrum of copper

2.3 Nickel Spectrum

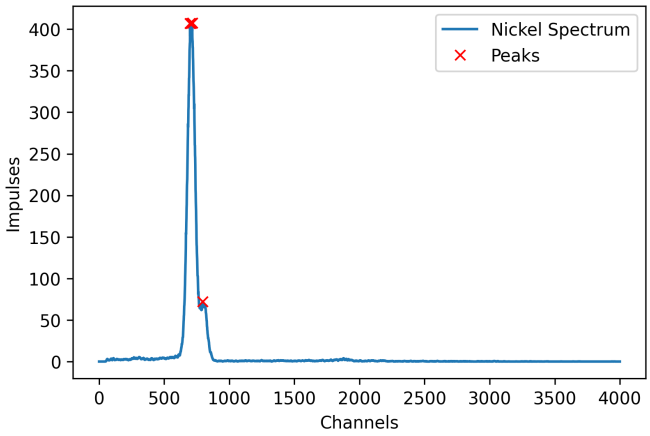

Figure 4: The X-ray emission spectrum of nickel

2.4 Titanium Spectrum

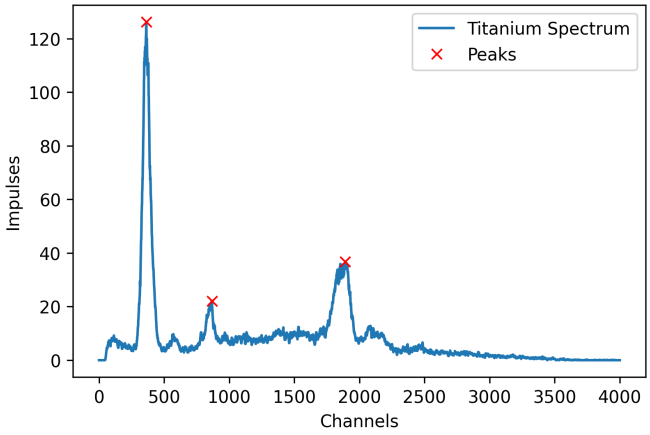

Figure 5: The X-ray emission spectrum of titanium

2.5 Unknown Source

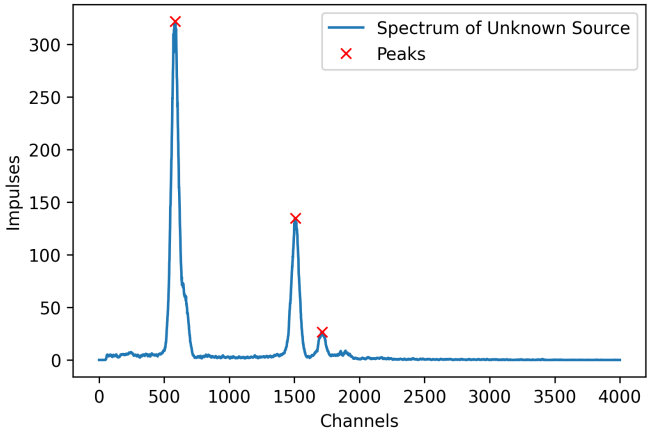

Figure 6: The X-ray emission spectrum of the unknown source

2.6 Israeli 10-Cent Coin Spectrum

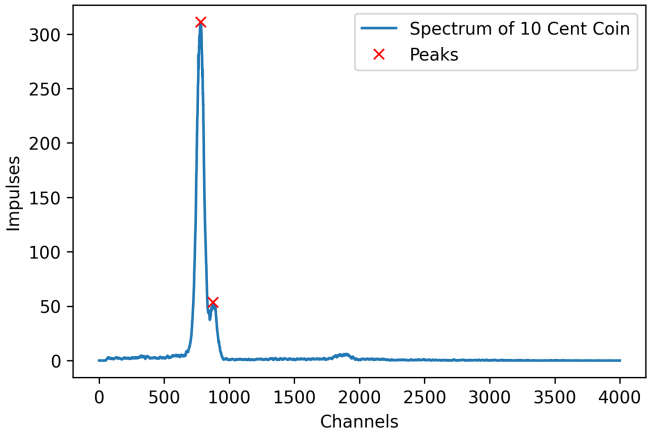

Figure 7: The X-ray emission spectrum of a 10 cent Israeli shekel coin

2.7 Strontianit Spectrum

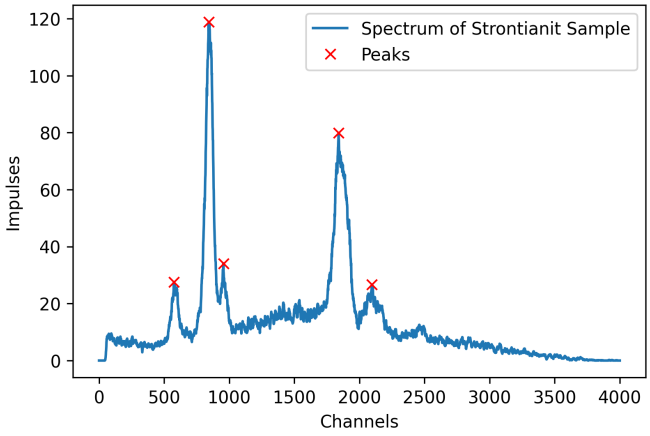

Figure 8: The X-ray emission spectrum of strontianit

2.8 Pyrrhotin Spectrum

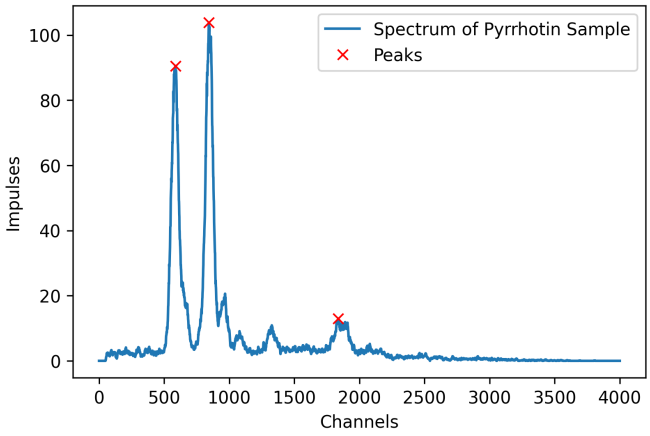

Figure 9: The X-ray emission spectrum of pyrrhotin

3 Analysis

3.1 Analysis of the Molybdenum Spectrum

Using the provided table, we were able to deduce that the three peaks found in Figure (2) were of energies 8027.8 eV, 8905.3 eV and 17479.3 eV respectively. The 8027.8 eV and 8905.3 eV both correspond to the X-ray emission lines of copper, while the 17479.3 eV corresponds to an emission line of molybdenum.

3.2 Analysis of the Copper Spectrum

Using the provided table, we were able to deduce that the two peaks found in Figure (3) were of energies 8027.8 eV and 8905.3 eV respectively. The 8027.8 eV and 8905.3 eV both correspond to the X-ray emission lines of copper, similar to the emission lines found in Figure (2).

3.3 Analysis of the Nickel Spectrum

Using the provided table, we were able to deduce that the two peaks found in Figure (4) were of energies 7460.9 eV, 8905.3 eV and 8264.7 eV respectively. These values all correspond to the X-ray emission lines of nickel.

3.4 Analysis of the Titanium Spectrum

Using the provided table, we were able to deduce that one of the peaks found in Figure (5) was of energy 4510.8 eV. This corresponds to the X-ray emission lines of titanium. The other peaks do not seem to correspond to the known spectrum of titanium, but rather to a small amount of copper that might have been present in the system.

3.5 Calibration of the System using Linear Regression

By plotting the energy values we obtained against the channel at which we achieved that energy value for all of the elements (molybdenum, copper, nickel and titanium), we were able to perform a linear regression which can be used in order to calculate the energy values and therefore elemental composition of other materials. This regression is shown in Figure (10) below. From this regression we calculated a slope of $a = 8.3$ and y-intercept $b = 1547.3$.

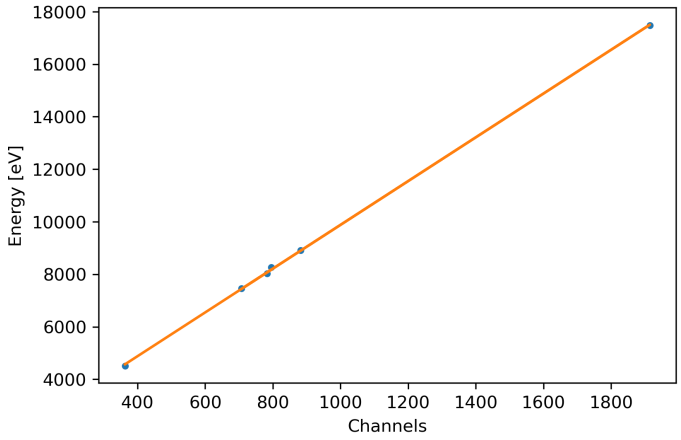

Figure 10: The X-ray emission spectrum of nickel

3.6 Analysis of the Emission Spectrum of the Unknown Source

As seen in Figure (6), we get three peaks at channels 583, 1508 and 1714. Using the linear regression, this corresponds to energy values of 6404.5 eV, 14111.2 eV and 15827.5 eV respectively. Looking at the table and taking into the sources found in the lab, it is most probable that the unknown source was sriconium. Sriconium has X-ray emission lines at 14165.0 eV and 15824.9 eV, which when compared to the emission lines calculated at 14111.2 eV and 15827.5 eV, yields χ^2 values of 0.2 and $4 \cdot 10^{-4}$ respectively.

We were not able to find an emission line of sriconium around 6404.5 eV. Therefore, we propose that this emission line actually comes from copper. However, the nearest copper emission is at 8047.8 eV, yielding a relatively high χ^2 value of 335.5.

3.7 Analysis of the Emission Spectrum of the 10 Cent Coin

As seen in Figure (7), we get two peaks at channels 779 and 875. Using the linear regression, this corresponds to energy values of 8037.5 eV, and 8837.3 eV respectively. According to [1], the composition of an Israeli 10 cent coin is 92 percent copper, 6 percent aluminium and 2 percent nickel. As such, it is likely that the calculated energy value of 8037.5 eV corresponds to the X-ray emission line of copper at 8027.8 eV. Additionally, the energy value of 8837.3 eV corresponds to the X-ray emission line of copper at 8905.3 eV. Performing chi squared analysis, we get errors of $\chi^2 = 0.01$ and $\chi^2 = 0.5$ respectively.

3.8 Analysis of the Emission Spectrum of Strontianit

As seen in Figure (8), we get five peaks at channels 575, 843, 955, 1840 and 2095. Using the linear regression, this corresponds to energy values of 6337.9 eV, 8570.8 eV, 9503.9, 16877.3 eV and 19001.8 eV respectively. According to [3], Strontianit is a crystal composed of sriconium, carbon and oxygen. Looking at the given table, we see that the 8570.8 eV corresponds to the copper spectral line at 8047.8 eV, yielding a χ^2 value of 33.9. Similarly, it is likely that the peak at 9503.9 eV corresponds to the X-ray emission line of copper at 8905.3 eV. This leads to a χ^2 value of 40.2. The peak at 16877.3 eV corresponds to the sriconium spectral line at 15835.7 eV, resulting in a χ^2 value of 68.5. The peak at 19001.8 eV probably corresponds to the spectral line of molybdenum at 19608.3 eV, leading to a χ^2 value of 18.8.

We were unable to determine the reason behind the peak at 6337.9 eV. It is possible that it corresponds to the copper emission line at 8027.8 eV, although this results in a relatively large χ^2 value of 355.73.

3.9 Analysis of the Emission Spectrum of Pyrrhotin

As seen in Figure (9), we get three peaks at channels 587, 843 and 1838. Using the linear regression, this corresponds to energy values of 6437.9 eV, 8570.8 eV and 16860.6 eV respectively. According to [2], Pyrrhotin is a crystal composed of iron and sulphur. Indeed, looking at the given table, we see that there is an X-ray emission line with a very high relative intensity (100) at 6403.8 eV. Comparing the calculated and theoretical values for this spectral line, we obtain a χ^2 value of 0.2. The other energy values obtained are not anywhere near the expected emission lines of iron and sulphur. As such, they are probably from molybdenum or copper. Molybdenum has a spectral line at 17374.3 eV, which is relatively close to 16860.6 eV. This gives us a χ^2 value of 15. Moreover, there is a copper spectral line at 8047.8 eV, which when compared to 8570.8 eV gives a χ^2 value of 33.9.

4 Conclusion

In this work, we measured the X-ray spectra of various materials and minerals in order to characterize new and unknown materials. We were able to use a set of known materials to calibrate the conversion between voltage readings and energy levels for the spectrum lines, and from there identify unknown sources as well as other known sources, including some minerals. Our linear fit for the calibration was satisfactorily good, and produced decent results (low χ^2 values) for the sources that we identified afterwards, however there were notable errors caused by the presence of other materials (such as copper and molybdenum) in the system. Additionally, the more complex sources - especially the Strontianit - produced some poorer results, either due to the complexity of the material or due even to a possible mislabeling of the source. Regardless, our experiment overall presented a worthwhile investigation into the world of X-ray spectroscopy.

References

[1] 10 agorot. https://en.numista.com/catalogue/pieces1715.html.

[2] Pyrrhotite. https://www.mindat.org/min-3328.html.

[3] Strontianite mineral data. http://webmineral.com/data/Strontianite.shtml.

Appendix A: Error Analysis

A.1 Standard Error of Linear Regression Slope

$$\sigma_\beta = \sqrt{\frac{1}{n-2} \cdot \frac{\Sigma(y_i - \hat{y}_i)^2}{\Sigma(x_i - \bar{x})^2}}$$

A.2 χ^2 Metric

$$\chi^2 = \sum_i \frac{(O_i - E_i)^2}{E_i}$$