# X-Ray Explorations: Fluorescence and Bragg Scattering

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We make measurements of  $K_{\alpha}$  and  $K_{\beta}$  X-ray emission lines for various metals ranging from atomic number Z = 22 to Z = 56. Using single and double Gaussian models, we fit fluorescence spectra of our samples to measure  $K_{\alpha}$ , finding agreement (for all but two of our samples) to literature values within 1 $\sigma$  of uncertainty. We also use our results to compare to Mosley's law for  $K_{\alpha}$  emission line energies, finding a quadratic model to be a reasonable fit to our data ( $\chi^2_{red} = 3.16$ ) and finding a best-fit parameter that agrees to the accepted value of 0.75hcR within  $2\sigma$  of uncertainty. We also use Bragg scattering for precise determination of Copper (Z = 29) X-ray emission energies, finding the  $K_{\alpha}$  line at  $7.87(16)_{sys}(1)_{stat}$  keV and the  $K_{\beta}$  line at  $8.78(20)_{sys}(2)_{stat}$  keV. We find both to be in agreement with litearture values within  $1.1\sigma$  of uncertainty, and also find the high-energy cutoff to be in consistent with experimental parameters.

## I. INTRODUCTION

X-ray spectroscopy is a broadly useful tool, for example in medical imaging as well as for the probing of electronic structure of atoms. In this paper, we consider the latter application, and use a Tel-X-Ometer spectrometer to measure the energies of x-rays produced through direct detection, fluorescence, and Bragg scattering. Through this, we aim to make precise enough measurements for meaningful comparison to literature values and test empirical laws that describe emission energies.

The rest of this paper is organized as follows. In Section II we introduce the necessarily theoretical background to understand our results. In Section III we give an overview of the experimental apparatus. In Section IV we provide our experimental results and analysis. In Section V we discuss our results and conclude with possibilities for future work.

#### II. THEORY

#### A. X-ray emission

There are two mechanisms that give rise to x-rays as a metal target is struck by energetic electrons. The first is a continuous spectrum known as Bremsstrahlung radiation, wherein all energies between 0 and  $E_{\text{max}} = eV - \Phi \approx eV$  (where eV is the energy of the incoming electron accelerated through voltage V, and  $\Phi$  is the work function of the metal, which we can neglect for accelerating voltages on the order of keV). This continuous spectrum has a high-energy cutoff given by:

$$\Delta_{\text{high}} = eV = \frac{hc}{\lambda} \tag{1}$$

wherein  $\lambda$  is the (minimum) emittable wavelength.

The second mechanism is discrete, and arises when the incoming electrons liberate the electrons of inner subshells of the atoms in the target metal. Such atoms are then unstable - electrons in higher shells then transition to the lower shells, releasing X-rays of discrete energy in the process. In this work, we particularly concern ourselves with the  $K_{\alpha}$  (corresponding to  $n = 2 \rightarrow n = 1$ or the L shell  $\rightarrow$  K shell transition) and the  $K_{\beta}$  (corresponding to  $n = 3 \rightarrow n = 1$  or the M shell  $\rightarrow$  K shell transition) lines.

The overall spectrum produced by a target emitting x-rays is the superposition of the continuous Bremsstrahlung and the discrete lines. In this work, we are interested in measuring these discrete emission lines as these are what give insight into the atom-specific structure.

#### B. X-ray fluorescence

One way the discrete emission lines can be probed is through fluorescence, wherein a material is exposed to xrays more energetic than the atomic binding energy. This has the effect of liberating low-energy electrons, wherein higher energy electrons transition into the vacant states, emitting/fluorescing a secondary x-ray. An empirical law that relates the emission energy E to the atomic number Z is given by Moseley's law:

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

where h is the Planck constant, c the speed of light, and R the Rydberg constant. In particular, this law models the energies of the  $K_{\alpha}$  line, and in our analysis we will test the validity of this empirical law.

## C. Bragg scattering

A high-resolution method for distinguishing X-rays of different energies is through Bragg scattering, wherein X-rays with specific energies constructively interfere and

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FIG. 1. Diagram of Tel-X-Ometer and supporting electronics, reproduced from the 334 lab wiki [1].

diffract from the crystal. The Bragg condition is given by:

$$n\lambda = 2d\sin\theta \tag{3}$$

Where *n* is the order of diffraction,  $\lambda$  is the wavelength of the x-ray (related to the energy of the x-ray by Eq. (1)), *d* is the crystal spacing, and  $\theta$  is the angle between the incident x-rays and the crystal surface. For a beam of x-rays composed of multiple different wavelengths, at fixed  $\theta$  only wavelengths obeying the Bragg condition are diffracted, giving rise to high energy resolution based on crystal orientation.

### **III. APPARATUS**

The experimental apparatus centers around a Tel-X-Ometer which comprises a (Copper) X-ray source and detector and supporting electronics (such as volto/ammmeters, ratemeters, a high-voltage supply, and amplifier). A diagram of the setup is provided in Fig. 1.

The X-rays are produced in the following manner; electrons are accelerated through a (tunable) acceleration voltage to a copper target, wherein the electrons are collimated towards the crystal post holder. For the fluorescence experiments, we mount the metal foils of interest on this central post and angle the carriage arm at 90 degrees such that the proportional counter only receives x-rays from the fluorescing metal. For the Bragg diffraction experiment, we mount a LiF crystal on the post, and then can rotate the the carriage arm to adjust the diffraction angle  $\theta$ , wherein only x-rays with wavelength/Energy obeying Eq. (3) are detected by the proportional counter.

The proportional counter contains Xenon and CO<sub>2</sub> surrounding a central wire. X-rays that enter the tube ionize the gas and release electrons, causing a cascade, with the magnitude of the pulse pulse proportional to the energy of the incidident electron. The pulse then produces a dip in the central wire voltage, producing a digital signal. This signal is amplified and sent to a digital pulse height analyzer (PHA), which forms the basis of the count vs. channel (energy) spectra which we analyze in this report. Before moving onto our results, we note a slight subtely in the data collection in that a overly high intensity of x-ray radiation results in a saturation of the proportional counter, wherein the voltage of the central wire does not have sufficient time to recover between detection events. This can result in a pulse being recorded at a lower energy than its actual energy, resulting in a shift in spectral features, which is a dangerous systematic effect if trying to extract energies from spectra. In order to avoid this saturation effect, we adjust the x-ray intensity (via slits/collimators or source distance/angle) such that the detector dead time (a measure of saturation) is never greater than 5%.

#### IV. RESULTS

### A. Fluorescence

#### 1. Calibration

We took data at two different acceleration voltages. studying Z = 23 - 30 metals at a 25kV setting and Z =22,37-56 metals at a 15kV setting (wherein we chose a smaller acceleration voltage for a greater PHA energy range). For each of these two settings, we must perform a calibration in order to convert between the PHA channel number to the energy of detected radiation. For each voltage setting, we performed a 3-point calibration. For both settings we use a direct Co-57 source, which emits a 14.4keV x-ray through electron capture to Fe-57 and a subsequent 6.4 keV x-ray from the  $K_{\alpha}$  line of Iron. For the 25kV setting we further use the 8.6keV  $K_{\alpha}$  line of Zn-64 and for the 15kV setting we further use the 32.2keV  $K_{\alpha}$ line of Ba-133, so as to calibrate over a sufficient range of energies. The relationship between the channel C and energy E is linear, and is determined by:

$$C = mE + b \tag{4}$$

where we obtain the reference/calibration E from [2], the channel C as the centroids of the emission peaks on the PHA (how these are determined are described in the next section), and the m, b are determined as best-fit parameters. The result of this calibration is given in Fig. 2



FIG. 2. Plot of calibration peak energies vs. channel centroids, along with linear calibration fits according to Eq. (4), with parameters given in Table. I. Error bars are statistical and arising from uncertainty in fit parameters, and are hidden behind markers.

Fit parameter	25keV accel. voltage	15keV accel. voltage
m (channel $\cdot \text{keV}^{-1}$ )	$55.71(43)_{\rm sys}(11)_{\rm stat}$	$26.04(43)_{\rm sys}(2)_{\rm stat}$
b (channel)	$12.7(35)_{\rm sys}(10)_{\rm stat}$	$34.8(35)_{\rm sys}(4)_{\rm stat}$

TABLE I. Best-fit calibration parameters relating PHA channel and energy.

In addition to the statistical uncertainty arising from the fit, there is also a systematic uncertainty associated with this calibration, which we characterize as arising from the drift in acceleration voltage/gain. In order to estimate this systematic, we repeated the measurements of the calibration peaks and the fitting procedure across the week in which fluorescence data was collected, and computed the fitting parameters m, b across multiple calibration sessions. Doing so, we find a standard deviation of  $\sigma_m = 0.43$ channels  $\cdot \text{keV}^{-1}$  and  $\sigma_b = 3.5$ channels, which we take as an estimate of our systematic uncertainty in our calibration parameters.

## 2. Fitting Peaks

To each spectra, in the region of interest we fit a Gaussian fitting function to the peak corresponding to the  $K_{\alpha}/K_{\beta}$  emission line. The resolution of our detector is insufficient to distinguish these emission lines as distinct peaks, and they generally appear as single peaks in the obtained spectra. When the peak exhibits symmetry, we fit the Gaussian with linear background given in Eq. (5).

$$M_1(x) = \frac{N}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(x-\mu)^2}{2\sigma^2}) + Bx + C \quad (5)$$

When the peak exhibits asymmetry due to the overlapping  $K_{\alpha}/K_{\beta}$  lines or or the peak is roughly symmetric but close to a contaminant peak, we fit to it a double Gaussian with linear background given in Eq. (6).

$$M_{2}(x) = \frac{N_{1}}{\sqrt{2\pi\sigma_{1}^{2}}} \exp(-\frac{(x-\mu_{1})^{2}}{2\sigma_{1}^{2}}) + \frac{N_{2}}{\sqrt{2\pi\sigma_{2}^{2}}} \exp(-\frac{(x-\mu_{2})^{2}}{2\sigma_{2}^{2}}) + Bx + C$$
(6)

The goodness of fit parameter being reasonable with a single Gaussian and/or the double Gaussian fit exhibiting degeneracy in the fitting parameters were used as indiciations to use the model in Eq. (5) over Eq. (6), but most of the spectra were better fit by the double Gaussian.

As an example, we provide the fitting of the  $K_{\alpha}$  peak of Iron using a double Gaussian fit in Fig. 3 below, wherein the asymmetry arising from the unresolved  $K_{\beta}$ peak makes the peak amenable to a double Gaussian fit. The channel corresponding to the  $K_{\alpha}$  peak is extracted from the fitting parameter  $\mu$  or  $\mu_1$ , and can then be converted into an energy via the described three-point calibration procedure. For brevity, all other fits are tabulated in Appendix A. We note that all peaks appear to be well-modeled either by single or double Gaussians, with  $\chi^2_{\rm red} < 2$  in all cases, except for Titanium where a contaminant (presumed to be Copper) peak interferes with the fit.

### 3. Measurement of $K_{\alpha}$ via Fluorescence

Repeating this fitting procedure for each metal of interest, we can obtain the peak centroids  $\mu$  which can then be converted from channels to energies using the linear calibration described in the previous section. This procedure yields a measurement of the  $K_{\alpha}$  emission line energy for each tested metal. Each of these energies has a statistical uncertainty arising from the fit (uncertainty in fitting the peak centroids) as well as a systematic uncertainty arising from calibration, which we separate. We tabulate all measured values of  $K_{\alpha}$  lines and associated uncertainties in Table. II below. We also tabulate the accepted literature value from [2] and compare the values via t'-statistic.

#### 4. Testing Mosley's Law

To test Mosley's dataset of  $K_{\alpha}$  emission line values, we fit a model of the form:

$$E(Z) = \epsilon (Z - 1)^2. \tag{7}$$

The our dataset. A plot of our measured  $K_{\alpha}$  vs. Z along with the best fit model is given in Fig. 4 below.



FIG. 3. Fitting of Iron (Z = 26) fluorescence spectra. The top plot is the full spectrum, and the bottom plot restricts to the region of interest (channels [250, 500]) with the emission peak. Data is in blue (with associated counting uncertainties  $\sqrt{N}$  arising from Poisson statistics) and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 5.3(11) \times 10^4$  counts,  $\mu_1 = 364.0(10)$ channel,  $\sigma_1 = 24.21(88)$ channel,  $N_2 = 1.2(1.1) \times 10^4$ counts,  $\mu_2 =$ 399.1(27)channel,  $\sigma_2 = 33.5(92)$ channel,  $B = 1.09(11) \times$  $10^{-2}$ counts/channel, C = -24.4(29)counts, with a reduced chi-squared of  $\chi^2_{red} = 1.02$ , indicating a good fit.

### B. Bragg Scattering

We set the electron acceleration voltage to 15kV. We varied the diffraction angle  $\theta$  from  $\theta = 35^{\circ}$  to  $\theta = 12^{\circ}$ so as to capture the  $K_{\alpha}, K_{\beta}$  peaks and the high energy cutoff of the spectra. We note there is a systematic uncertainty of  $\theta = 0.5^{\circ}$  associated with calibrating the orientation of crystal at zero degrees. At each angle, we fit the spectra using a Gaussian with linear background Eq. (5) and obtain the count rate  $R = \frac{N}{T}$  from the fitting parameter (number of counts) N and the data collection time T. The uncertainty in R can be obtained by adding the statistical uncertainty in the fit parameter N and the timing resolution uncertainty T (0.5s) in quadrature. An

Z	Element	Best Fit $(keV)$	Literature (keV)	t'
22	Ti	$3.63(16)_{\rm sys}(2)_{\rm stat}$	4.511	5.48
23	V	$4.78(20)_{\rm sys}(2)_{\rm stat}$	4.952	0.82
24	$\operatorname{Cr}$	$5.29(21)_{\rm sys}(2)_{\rm stat}$	5.414	0.60
25	Mn	$5.80(21)_{\rm sys}(2)_{\rm stat}$	5.898	0.46
26	Fe	$6.38(21)_{\rm sys}(2)_{\rm stat}$	6.403	0.10
27	Co	$6.96(21)_{\rm sys}(2)_{\rm stat}$	6.903	0.28
28	Ni	$7.55(21)_{\rm sys}(3)_{\rm stat}$	7.478	0.35
29	Cu	$8.12(21)_{\rm sys}(3)_{\rm stat}$	8.0947	0.13
30	Zn	$8.65(21)_{\rm sys}(3)_{\rm stat}$	8.638	0.06
37	$\operatorname{Rb}$	$13.28(28)_{\rm sys}(3)_{\rm stat}$	13.395	0.42
41	Nb	$17.06(33)_{\rm sys}(4)_{\rm stat}$	16.615	1.32
42	Mo	$17.53(34)_{\rm sys}(3)_{\rm stat}$	17.479	0.15
47	Ag	$22.23(41)_{\rm sys}(3)_{\rm stat}$	22.162	0.16
56	Ba	$31.98(57)_{\text{sys}}(3)_{\text{stat}}$	32,193	0.37

TABLE II. Measured values of  $K_{\alpha}$  emission lines from peak fitting + conversion to energies via calibration, alongside literature values from [2]. A t'-statistic is provided comparing the measured and literature value.



FIG. 4. Plot of  $K_{\alpha}$  vs. Z data from Table. II along with best-fit curve with model Eq. (7). The plotted error bars are systematic as these are the dominant (by factor 10x) uncertainty in the obtained  $K_{\alpha}$  energy values. We magnify the error bars by 2x (they represent  $\pm 2\sigma$ ) for greater visibility. The fit has a reduced chi-squared of  $\chi^2_{\rm red} = 3.16$  and best-fit parameter of  $\epsilon = 10.310(69)_{\rm stat}$  eV.

example of such a fit is given in Fig. 5.

We chose the angular spacings between datapoints to be fine where the rate was rapidly changing (i.e. in the vicinity of the  $K_{\alpha}/K_{\beta}$  peaks and the high energy cutoff) and coarse where the rate did not change appreciably with angle. Computing the rate at each angle, we obtain the top plot of Fig. 6. We can then convert the angles  $\theta$ into energies through the Bragg diffraction equation Eq. (3), considering the first order diffraction peak n = 1 and using the provided LiF crystal spacing from [3]:

$$d = 0.2008(1)$$
nm (8)

to obtain the bottom plot of Fig. 6.





FIG. 5. Fitting of Copper Bragg Diffraction spectra. The top plot is the full spectrum, and the bottom plot restricts to the region of interest (channels [300, 575]) with the Bragg diffraction peak peak. Data is in blue (with associated counting uncertainties  $\sqrt{N}$  arising from Poisson statistics) and best fit of a single Gaussian with linear background (Eq. (5)) is in red, Best fit parameters are found to be  $N_1 = 8.534(31) \times 10^4$ counts,  $\mu_1 = 431.81(10)$ channel,  $\sigma_1 = 25.505(76)$ channel,  $B = -5.64(31) \times 10^{-2}$ counts/channel, C = 32.3(16)counts, with a reduced chi-squared of  $\chi^2_{\rm red} = 1.07$ , indicating a good fit.

From the data in Fig. 6, the value for the  $K_{\alpha}, K_{\beta}$  lines is estimated to be the energy (angle) at which the count rate is maximized. Since the peaks are sharp, we estimate the statistical uncertainty in this peak estimation as a quarter of the angular resolution of our collected data, or 0.04°. The 0.5° angular systematic uncertainty arising from the calibration is relatively large to this, and hence is the limiting uncertainty. This angular uncertainty can be converted into energy uncertainty via the derivative of Eq. (3). We thus obtain the final values as in table Tab. III, where we also give the literature values from [2].

We can also estimate the high-energy cutoff from where the count rate falls to that indistinguishable from background, which occurs at:

$$\Delta_{\rm high} = 14.84(60)_{\rm sys}(5)_{\rm stat} {\rm keV}.$$
 (9)



FIG. 6. (Top): Semi-log plot of diffraction angle  $\theta$  vs. count rate. Error bars in count rate are statistical and determined from uncertainty in fitting parameters. The error in angle is omitted from the plot for clarity. (Bottom): Semi-log plot of energy vs. count rate, converted from angle using Eq. (3). The emergence of the  $K_{\alpha}, K_{\beta}$  emission peaks, as well as the high-energy cutoff can be observed. For comparison, the literature values [2] of the  $K_{\alpha}/K_{\beta}$  emission lines are overlayed on the plot as vertical lines.

Em. Line	Measured (keV)	Literature (keV)	ť'
$K_{\alpha}$	$7.88(16)_{\rm sys}(1)_{\rm stat}$	8.047	1.1
$K_{\beta}$	$8.78(20)_{\rm sys}(2)_{\rm stat}$	8.905	0.59

TABLE III. Measured values for the  $K_{\alpha/\beta}$  emission lines of Cu, and comparison to literature [2] values.

## V. DISCUSSION

In the fluorescence measurements, we find that all measurements of  $K_{\alpha}$  agree with the literature values to within  $1\sigma$ , with the exception of Nb (which agrees within  $1.5\sigma$ ) and Ti, which disagrees with t' = 5.48. Studying the fit of the Titanium data in Fig. 21, we find that the contaminant copper peak interferes with the fit, possibly leading to an unreliable estimation of the  $K_{\alpha}$  centroid for Ti. A four-Gaussian model that capture the  $K_{\alpha}/K_{\beta}$  peaks of both Ti/Cu may better fit the data and allow for a more accurate determination of the  $K_{\alpha}$  line of Ti.

Using our  $K_{\alpha}$  fluorescence data to test the validity of Mosley's Law, we find that our data is well-fit by the functional form  $E(Z) = \epsilon(Z-1)^2$ , with a reduced chisquared of  $\chi^2_{\rm red} = 3.16$ . In addition, the best-fit parameter yields  $\epsilon = 10.310(69)_{\text{stat}}eV$ , which is in  $2\sigma$  of agreement with the coefficient coefficient 0.75hcR = 10.20eV as predicted by Mosley's law. Our data is thus consistent with it. As Mosley's law is phenomelogical rather than fundamental, as we reach higher precision in our  $K_{\alpha}$ measurements we would expect to see deviations from its predictions. Future experiments could seek to increase the precision in the  $K_{\alpha}$  measurements to reach a regime where the law can be challenged. Our dominant source of uncertainty is systematic, arising from the drift in gain voltage which affects the energy calibration and subsequent values. A future experiment could determine individual  $K_{\alpha}$ s by calibrating in between every measurement cycle to prevent the effects of such a systematic drift. Our investigations for fluorescence focused on the  $K_{\alpha}$  line, but a future experiment with a higher-energy resolution detector (wherein the  $K_{\alpha/\beta}$  peaks in our fluorescence data could be resolved) may explore the functional form of the  $K_{\beta}$  emission lines, or look at higher order transitions (e.g. the L/M-lines not studied in this work).

In the Bragg scattering experiment, we found  $K_{\alpha}, K_{\beta}$ energies for Copper that were in agreement with the literature, with the  $K_{\alpha}$  value in agreement to  $1.1\sigma$  and the  $K_{\beta}$  value in agreement below  $1\sigma$ . We also find a high energy cutoff value which is in agreement to  $1\sigma$  to the experimental parameter of 15kV accelerating voltage, serving as an internal consistency check to the experiment. The uncertainty in these values were dominated by the systematic uncertainty associated with the zeroangle alignment with the crystal. The most obvious improvement for a future experiment would be to decrease this systematic uncertainty, e.g. improving the crystal alignment using lasers. A future experiment could also do two sets of Bragg scattering experiments using distinct X-ray sources, one to independently verify/calibrate the LiF crystal spacing, and the second to measure the emission energies using the measured spacing (as using the obtained copper  $K_{\alpha}/K_{\beta}$  energies to measure d would be circular - we require a distinct energy reference).

### DATA AVAILABILITY

The raw data as well as the Jupyter notebook used for data analysis can be found in the attached rioxray.zip file, submitted along with this report.

## Appendix A: Fits of Fluorescence Spectra

In this Appendix, we provide the individual fits of the fluorescence spectra from which the  $K_{\alpha}$  emission energies in the main text were derived. All error bars in plots arise

from the  $\sqrt{N}$  Poissonian statistical counting uncertainty. Uncertainties in fitting parameters provided in captions are statistical and originate from the fit. Fitting parameters N, C are measured in counts,  $\mu, \sigma$  are measured in channels, and B is measured in counts/channel. The relevant fitting parameter that was extracted from these fits to convert to the peak energy was the peak centroid  $\mu$ .

### 1. 25keV Dataset



FIG. 7. Full spectrum from direct Cobalt (Z = 27) source, used for calibration of 15kV dataset.



FIG. 8. Fitting of first peak of direct Cobalt (Z = 27) spectra for calibration. Data is in blue and best fit of Gaussian (corresponding to unresolved  $K_{\alpha}/K_{\beta}$  emission peak of Fe - 57) with linear background (Eq. (5)) is in red. Best fit parameters are found to be  $N = 1.953(16) \times 10^4$ ,  $\mu = 368.73(24)$ ,  $\sigma = 27.05(21)$ ,  $B = 2.4(19) \times 10^{-3}$ , C = 5.79(78), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.01$ .



FIG. 9. Fitting of second peak of direct Cobalt (Z = 27) spectra for calibration. Data is in blue and best fit of Gaussian (corresponding to Co-57  $\rightarrow$  Fe-57 decay) with linear background (Eq. (5)) is in red. Best fit parameters are found to be  $N = 5.41(15) \times 10^3$ ,  $\mu = 814.24(87)$ ,  $\sigma = 38.71(95)$ ,  $B = 1.5(38) \times 10^{-3}$ , C = 2.2(34), with a reduced chi-squared of  $\chi^2_{\rm red} = 0.66$ .



FIG. 10. Fitting of Zinc (Z = 30) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 2.71(28) \times 10^4$ ,  $\mu_1 = 488.43(68), \sigma_1 = 26.56(81), N_2 = 2.63(2.7) \times 10^4$ ,  $\mu_2 = 504.4(16), \sigma_2 = 42.1(11), B = 2.51(39) \times 10^{-2},$ C = -1.6(23), with a reduced chi-squared of  $\chi^2_{\rm red} = 0.80$ .



FIG. 11. Fitting of Vanadium (Z = 23) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the (unresolved)  $K_{\alpha}/K_{\beta}$  peak and the second Gaussian fitting a contaminant peak. Best fit parameters are found to be  $N_1 = 7.472(29) \times 10^4$ ,  $\mu_1 = 279.22(10)$ ,  $\sigma_1 = 23.232(77)$ ,  $N_2 = 8.57(14) \times 10^3$ ,  $\mu_2 = 458.54(47)$ ,  $\sigma_2 = 28.17(45)$ ,  $B = 6.02(20) \times 10^{-2}$ , C = -2.48(82), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.66$ .



FIG. 12. Fitting of Chromium (Z = 24) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the (unresolved)  $K_{\alpha}/K_{\beta}$  peak and the second Gaussian fitting a contaminant peak. Best fit parameters are found to be  $N_1 = 2.621(18) \times 10^3$ ,  $\mu_1 = 307.45(18)$ ,  $\sigma_1 = 24.07(15)$ ,  $N_2 = 7.80(14) \times 10^2$ ,  $\mu_2 = 463.65(56)$ ,  $\sigma_2 = 31.66(55)$ ,  $B = 6.08(17) \times 10^{-2}$ , C = -7.35(55), with a reduced chi-squared of  $\chi^2_{\rm red} = 0.99$ .



FIG. 13. Fitting of Manganese (Z = 25) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the (unresolved)  $K_{\alpha}/K_{\beta}$  peak and the second Gaussian fitting a contaminant peak. Best fit parameters are found to be  $N_1 = 6.969(32) \times 10^4$ ,  $\mu_1 = 335.71(13)$ ,  $\sigma_1 = 25.21(10)$ ,  $N_2 = 1.574(70) \times 10^4$ ,  $\mu_2 = 456.80(78)$ ,  $\sigma_2 = 43.3(13)$ ,  $B = 4.1(14) \times 10^{-2}$ , C = 1.8(32), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.57$ .



FIG. 14. Fitting of Cobalt (Z = 27) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$ peak. Best fit parameters are found to be  $N_1 = 5.3(11) \times 10^4$ ,  $\mu_1 = 364.0(10), \ \sigma_1 = 24.21(88), \ N_2 = 1.2(1.1) \times 10^4,$  $\mu_2 = 399.1(27), \ \sigma_2 = 33.5(92), \ B = 1.09(11) \times 10^{-2},$ C = -24.4(29), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.02$ .



FIG. 15. Fitting of Nickel (Z = 28) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 3.71(21) \times 10^4$ ,  $\mu_1 = 427.1(15), \sigma_1 = 26.95(58), N_2 = 6.7(21) \times 10^3, \mu_2 =$  $474.5(63), \sigma_2 = 25.3(22), B = 2.71(31) \times 10^{-2}, C = -4.5(13),$ with a reduced chi-squared of  $\chi^2_{\rm red} = 0.76$ .



FIG. 16. Fitting of Copper (Z = 29) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 2.59(23) \times 10^4$ ,  $\mu_1 = 458.57(55), \sigma_1 = 25.41(68), N_2 = 1.77(23) \times 10^4, \mu_2 =$  $478(22), \sigma_2 = 37.79(82), B = 2.73(22) \times 10^{-2}, C = -5.94(95),$ with a reduced chi-squared of  $\chi^2_{\rm red} = 0.81$ .

## 2. 15keV Dataset



FIG. 17. Full spectrum from direct Cobalt (Z = 27) source, used for calibration of 15kV dataset.

FIG. 19. Fitting of second peak of direct Cobalt (Z = 27) spectra for calibration. Data is in blue and best fit of Gaussian (corresponding to Co-57  $\rightarrow$  Fe-57 decay) with linear background (Eq. (5)) is in red. Best fit parameters are found to be  $N = 1.018(13) \times 10^4$ ,  $\mu = 422.40(26)$ ,  $\sigma = 20.02(23)$ ,  $B = -4.8(34) \times 10^{-3}$ , C = 16.2(17), with a reduced chi-squared of  $\chi^2_{\rm red} = 0.92$ .

Channel

Counts



FIG. 18. Fitting of first peak of direct Cobalt (Z = 27) spectra for calibration. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 2.21(28) \times 10^4$ ,  $\mu_1 = 183.39(38)$ ,  $\sigma_1 = 12.08(41)$ ,  $N_2 = 1.75(27) \times 10^4$ ,  $\mu_2 = 193.1(14)$ ,  $\sigma_2 = 17.31(35)$ ,  $B = -2.21(74) \times 10^{-2}$ , C = 23.7(17), with a reduced chisquared of  $\chi^2_{\rm red} = 0.84$ .



FIG. 20. Fitting of Barium (Z = 56) fluorescence spectra for calibration. Data is in blue and best fit of Gaussian with linear background (Eq. (5)) is in red. Best fit parameters are found to be  $N = 4.190(36) \times 10^4$ ,  $\mu = 867.85(33)$ ,  $\sigma = 44.52(34)$ ,  $B = 2.036(56) \times 10^{-1}$ , C = -110.8(41), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.31$ .



FIG. 21. Fitting of Titanium (Z = 22) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the (unresolved)  $K_{\alpha}/K_{\beta}$  peak and the second Gaussian fitting the contaminant copper  $K_{\alpha}/K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 2.9153(84) \times 10^5$ ,  $\mu_1 = 1229.43(10)$ ,  $\sigma_1 = 11.289(27)$ ,  $N_2 = 3.4392(89) \times 10^5$ ,  $\mu_2 = 178.61(10)$ ,  $\sigma_2 = 21.116(61)$ ,  $B = 1.28(14) \times 10^{-2}$ , C = 168.5(30), with a reduced chi-squared of  $\chi^2_{\rm red} = 21.62$ .



FIG. 23. Fitting of Niobium (Z = 41) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 3.92(52) \times 10^4$ ,  $\mu_1 = 479.16(89), \sigma_1 = 23.2(84), N_2 = 3.6(11) \times 10^4$ ,  $\mu_2 = 410.8(24), \sigma_2 = 42(11), B = -2.265(78) \times 10^{-1},$ C = 1357(46), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.28$ .



FIG. 22. Fitting of Rubidium (Z = 37) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 9.65(32) \times 10^4$ ,  $\mu_1 = 380.63(48), \sigma_1 = 19.21(24), N_2 = 2.52(31) \times 10^4, \mu_2 = 420.8(27), \sigma_2 = 22.6(1.3), B = 3.17(40) \times 10^{-1}, C = -52(18)$ , with a reduced chi-squared of  $\chi^2_{\rm red} = 1.06$ .



FIG. 24. Fitting of Molybdenum (Z = 42) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 7.02(12) \times 10^4$ ,  $\mu_1 = 491.35(37), \sigma_1 = 22.85(19), N_2 = 1.67(12) \times 10^3$ ,  $\mu_2 = 545.3(21), \sigma_2 = 27.6(1.1), B = -7.63(52) \times 10^{-2}, C = 63.9(26)$ , with a reduced chi-squared of  $\chi^2_{\rm red} = 0.89$ .



FIG. 25. Fitting of Silver (Z = 47) fluorescence spectra. Data is in blue and best fit of double Gaussian with linear background (Eq. (6)) is in red, with the first Gaussian fitting the  $K_{\alpha}$  peak and the second Gaussian fitting the  $K_{\beta}$  peak. Best fit parameters are found to be  $N_1 = 6.781(49) \times 10^4$ ,  $\mu_1 = 613.76(28), \sigma_1 = 29.66(20), N_2 = 9.16(45) \times 10^3$ ,  $\mu_2 = 692.3(14), \sigma_2 = 27.11(98), B = -1.40(33) \times 10^{-2}$ , C = 32.3(18), with a reduced chi-squared of  $\chi^2_{\rm red} = 1.84$ .

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