X-ray Fluorescence and Moseley's Law

1 Background

1.1 Ordering of the periodic table

The 19$^{\text{th}}$ century saw many efforts to arrange the elements in a sensible order. The chemist John Dalton prepared one of the first tables of the elements in 1803, ordering them by increasing atomic weight. In the following decades it was recognized that groups of elements like lithium, sodium and potassium shared similar chemical properties, suggesting the presence of recurring patterns of chemical behavior. Using this concept, Dmitri Mendeleev developed around 1870 what is now known as the periodic table. Elements were placed in order in the periodic table, largely according to their atomic weight, and numbered consecutively, although no physical meaning was attached to these "atomic numbers." But this scheme had some puzzling anomalies, one of which was the ordering of nickel and cobalt; cobalt has higher atomic weight (58.93) than nickel (58.69), but its chemical properties suggest that it should precede nickel in the periodic table. This anomaly and others (atomic weight of argon is greater than that of potassium, same for tellurium and iodine) were gradually leading to the realization that the significant parameter in terms of ordering the periodic table was not atomic weight but rather the number of electrons and therefore the number of positive charges in the atom. A definitive resolution of these anomalies would await the X-ray measurements of H. G. Moseley.

In 1897 J. J. Thomson discovered the electron and established its discrete nature. The atomic model built on this discovery (the so-called raisin-pudding model) was one with positive charge distributed continuously throughout the atom with the electrons located at equilibrium positions in the atom, about which they oscillated when perturbed. Ernest Rutherford's alpha particle scattering measurements put this model to rest, as they demonstrated that the positively charged part of the atom consisted of a small, dense core, later termed the nucleus. In 1913 Niels Bohr, working in Rutherford's laboratory in Manchester, England, proposed a theory of the atom which combined Rutherford's results with the concept of quantized radiation developed by Planck and Einstein. In Bohr's model, the electron moves about the nucleus in a circular orbit, the attractive force resulting from the Coulomb interaction between the negatively charged electron and a nucleus with equal and opposite charge. The key breakthrough in Bohr's model was the quantization of electron angular momentum. Using this model, Bohr was able to derive the formula for wavelength of the light for the various transitions (also known as lines) in hydrogen-like spectra,

$$\frac{1}{\lambda} = R \left[\frac{1}{n_f^2} - \frac{1}{n_i^2} \right] Z^2. \tag{1}$$

The integers n_i and n_f represent the angular momentum (units of $\hbar$) of the initial and final states of the electron, and Z is an integer, known as the atomic number, representing the units of charge in the nucleus. R is the Rydberg constant; $R_\infty = me^4/4\pi c\hbar^3$, where m and e are the electron mass and charge, respectively, with the subscript denoting that this formula applies to an infinitely heavy nucleus. For a nucleus of finite mass M, the electron's mass m must be replaced by its reduced mass, $mM/(m + M)$.

Not only did the Bohr model accurately describe the spectrum of the hydrogen atom where $Z = 1$, but also for the singly ionized helium atom where one electron orbits a nucleus with $Z = 2$. The

success of the Bohr formula with the hydrogen and helium atoms suggested that it may also apply to transitions in heavier elements. If this proved to be the case, one would be able to order such transitions as a function of Z, thus providing an unambiguous means of ordering the elements in the periodic table.

The stage is now set for Moseley's measurements. It was already known that atoms of a given element emitted X-rays at well defined, characteristic energies. Armed with the new Bohr model, Moseley set about to measure the characteristic wavenumbers, $1/\lambda$, (inverse wavelengths, also proportional to frequency) for a number of different elements, and to correlate the X-ray frequency for a given element with the atomic number, Z, of that element.

Moseley's measurements were spectacularly successful. In the words of Robert Millikan (of Millikan oil drop/electron charge fame):

> "In a research which is destined to rank as one of the dozen most brilliant in conception, skillful in execution, and illuminating in results in the history of science, a young man twenty-six years old threw open the windows through which we could glimpse the sub- atomic world with a definiteness and certainty never dreamed of before."

Moseley's life was cut tragically short—he was killed at age 27 fighting for the British in World War I.

By measuring the wavenumber associated with a particular line (now designated K), from the spectrum of each element, Moseley established that the lines from a large number of elements obeyed the relation

$$\frac{1}{\lambda} = C(Z - \sigma)^2. \tag{2}$$

This relation is now known as Moseley's Law. C and σ are constants with $C \propto R$ (Rydberg constant) and $\sigma \approx 1$. σ is known as the screening constant. The connection between this formula and the Bohr formula is that $1/\lambda \propto Z^2$ in both cases. A plot representing Moseley's data is shown in Fig. 1. The data can be interpreted as resulting from an electron transitioning from an initial state with $n = 2$ to a final state with $n = 1$, with one other electron screening the nucleus, thus reducing the effective nuclear charge to $Z \approx 1$. An understanding of why the nucleus is screened by only one electron for the K lines would await the development of quantum mechanics in the 1920's.

Moseley's work provided an unambiguous justification for ordering the elements in the periodic table according to atomic number Z, rather than Mendeleev's original ordering by atomic weight A. His work helped resolve several outstanding problems with the table as it had existed: the above mentioned anomalies with heavier elements preceding lighter elements; the assignment of $Z = 44$ to ruthenium, implying that the element $Z = 43$ (technetium, which has no stable isotopes and must be synthesized in a nuclear reactor or particle accelerator) was as yet undiscovered; and the prediction of other as yet undiscovered elements at $Z = 61$, 72 and 75 [1].

With each element emitting X-rays at unique wavenumbers, X-ray analysis has become a powerful tool for analyzing chemical composition. X-ray analysis is used to determine the elements present in biological, environmental and geological samples. Figure 2 shows the X-ray spectrum from a water pollution sample, with channel number on the x-axis being proportional to X-ray energy, and the y axis showing the intensity of the detected X-rays. An X-ray detector very similar to the one you will use in this experiment was used on the Mars Sojourner Rover to analyze the composition of Martian rocks and soil. A spectrum obtained on this mission is available in the manufacturer's literature.
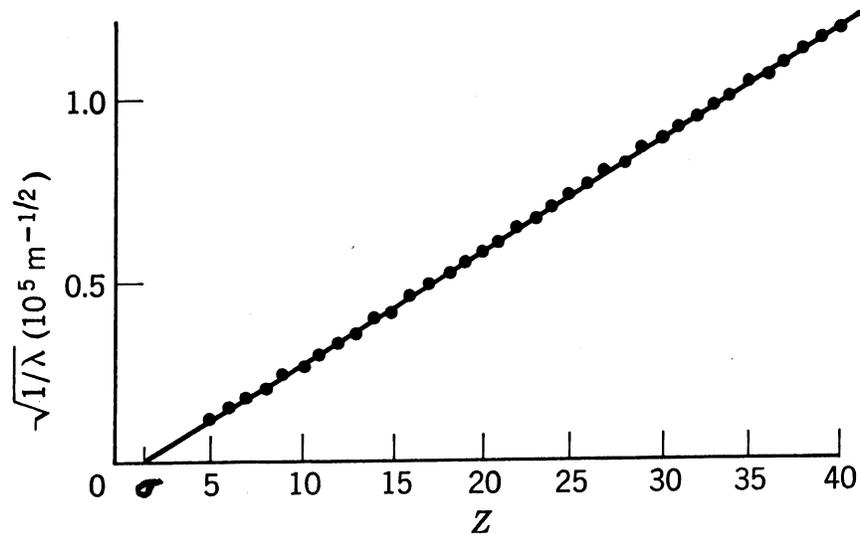
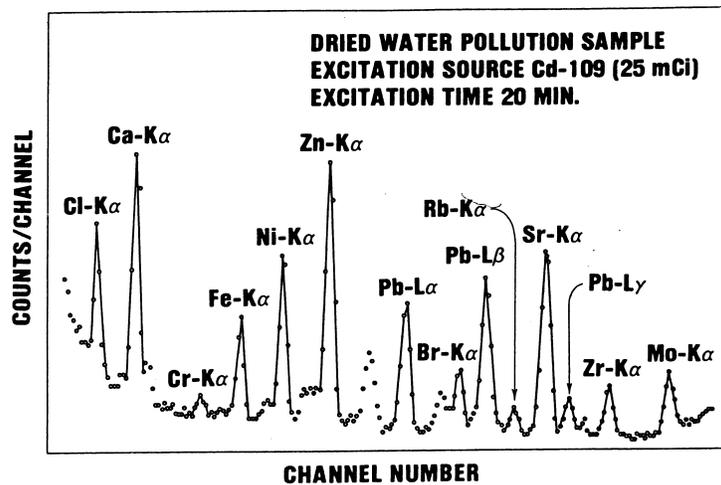Figure 1: Moseley's data. The line represents a fit to data using Moseley's Law.

Figure 2: X-ray spectrum of a water pollution sample.

As an aside, X-ray energy is obtained from wavenumber $1/\lambda$ by multiplication with hc where h is Planck's constant and c is the speed of light; remember $E =$ energy $= h\nu$ (Greek "nu") and $\nu = c/\lambda$.

1.2 Designations of the various X-rays

Moseley selected out one particular line, or energy, from the spectrum of each element to make the plot in Fig. 1. This is to say that there are more than one X-ray line associated with each element. This can be understood in terms of electrons transitioning between the various inner shells within the atom. Each shell is designated by a quantum number n, and an associated letter; $n = 1$, the innermost shell, is known as the K shell, $n = 2$ is known as the L shell, $n = 3$ is known as the M shell, and so on. Fig. 3 shows the possibilities for various transitions (vertical scale not linear – closer to logarithmic). The open arrows pointing upward represent electron transitions from the $n = 1$, $n = 2$, etc. levels to the cross-hatched region known as the continuum, where electrons are no longer bound to the atom. Such a transition results in a vacancy in the electron shell structure. The vacancy is filled when an electron from an higher lying shell (higher means greater n) transitions to a lower lying shell, accompanied by the emission of a characteristic X-ray. All transitions to the K shell are known as K lines, with the transition from the L shell known as the K_α line, from the M shell as the K_β line, and so on. Transitions to the L shell are known as L lines, and transitions to the M shell are known as M lines. The K lines are clearly more energetic than the L lines, and the K lines more energetic than the M lines.
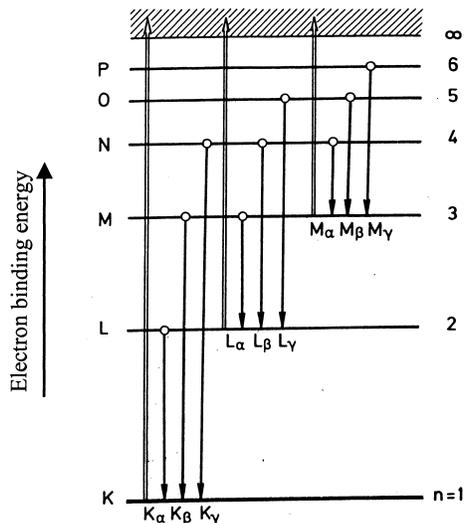

Figure 3: Diagram of K, L, M, etc. shell energy levels and identification of the various X-ray lines.

Within a given series of lines, K for example, the α line will clearly have less energy than the β line, and the β line less energy than the γ line. Many of the lines have sub-levels resulting from spin-orbit coupling and from screening effects [2]. These various levels are denoted by numerical subscripts, e.g. $K_{\alpha 1}$, $K_{\alpha 2}$. The energy differences between these sublevels are quite small for the lower Z elements. For iron ($Z = 26$) the $K_{\alpha 1}$ and $K_{\alpha 2}$ energies are 6.403 and 6.390 keV, respectively. This energy difference is too small to be resolved by our detector. At higher Z, the energy differences become appreciable; for lead, the $K_{\alpha 1}$ and $K_{\alpha 2}$ energies are 74.957 and 72.794 keV, respectively.

This splitting into sublevels is known as the "fine structure" of X-ray spectra.

Usually the K_α line is the most prominent feature of an X-ray spectrum. The K_β line will typically have 10-15% of the intensity of the K line for $Z \leq 30$, with the intensity ratio increasing to about 30% for the higher Z elements. A spectrum showing the K_α and K_β lines for a manganese target is shown in Fig. 4. For lower Z elements, identifying the K lines is usually the easiest way to determine the composition of a target; the L lines for these elements have very little energy and may not be detected efficiently by the detector, if detected at all. At higher X-ray energies the detector efficiency drops off so much (see attached efficiency curve for our detector) that the K lines for the higher Z elements will be hard to see. In this case, it may be easier to identify a high Z target by looking for its (lower energy) L lines, which are more efficiently measured by the detector.

1.3   How X-rays are generated

X-rays are photons with energy in the range of approximately 1 keV to 100 keV with corresponding wavelengths of approximately 1 nm to .01 nm. As mentioned previously, an X-ray results when an electron transitions between inner shells of an atom. For such a transition to occur, there must be a vacancy in one of the inner shells to which an electron can transition. How is such a vacancy created? There are three different ways: bombardment of the target with fast electrons; irradiation of the target with highly energetic photons, and by radioactive decay. In the first two cases, the particle striking the target must have sufficient energy to overcome the binding energy of the ejected electron. With electron bombardment, a sufficiently energetic electron striking the target can eject an inner shell electron from a target atom, thus creating the vacancy; this is how X-rays are generated in medical and dental X-ray machines. In the second case, an inner shell electron is also ejected, but this time by a sufficiently energetic photon. In the third case, a "parent" nucleus changes from Z to $Z - 1$ by capturing an electron from the innermost (K) shell, thus leaving a vacancy in the electron shell structure of the "daughter" atom. (This mode of radioactive decay is known as electron capture.)

In our apparatus, X-rays are produced by bombarding a target with energetic photons, namely, gamma rays. These photons result from the radioactive decay of ^{57}Co to ^{57}Fe by electron capture. After the decay, the daughter ^{57}Fe nucleus is left in an excited state, and it decays to the ground state by emitting photons with energy of 122 keV and 14 keV (and sometimes a single photon with energy 136 keV). Note the usage: photons which originate in the nucleus are called "gamma rays" even if their energy is the same as those arising from transitions in the electron shell ("X-rays"), as is the 14 keV mentioned. The ^{57}Fe atom also emits an X-ray as the K shell vacancy in the ^{57}Fe atom is filled. You may see these peaks in your spectra as well as the characteristic peaks coming from your sample.
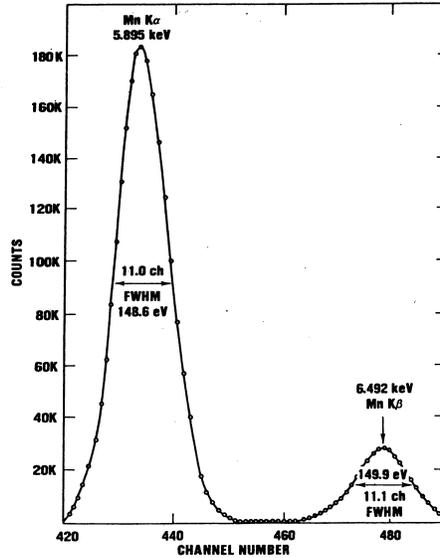
Figure 4: X-ray spectrum from a manganese target.

2   The experiment

Experimental Goal 1: Demonstrate a version of Moseley's Law with a detector that converts photon energy to peak voltage of an electronic pulse by studying a set of known samples. Establish the relationship given in Eq. (2), for which the peak voltage V is proportional to $1/\lambda$. Use these measurements to determine the screening constant σ for the K x-rays.

Experimental Goal 2: Determine the Z, and subsequently the element name, of six "unknown" samples in two ways:

1. From your Moseley's Law result, convert the measured peak voltages directly to Z.

2. First convert your voltage measurements to energy measurements using a look-up table for the known x-ray energies of your known samples. This will create a "calibration curve" for your instrument. Then feed in the measured voltages from the unknowns to determine measured energies. Use these and the look-up table to establish the elements. (This second method is the modern approach to spectroscopy.)

In this experiment, we bombard elemental samples with gamma radiation from a radioactive source to induce x-ray fluorescence. The x-rays emitted by the sample are detected by a solid state radiation detector, which produces electronic pulses whose amplitudes are proportional to the energy of the absorbed x-rays. Digitization electronics and a PC are used to record the pulses and histogram their amplitudes (in Volts) for subsequent analysis.

The known samples, in order of increasing Z, are listed in Table 1. Before starting, run the apparatus for 10–30 minutes without a target to use as a comparison for runs with a target in place. You want to be able to see the peaks which constitute the "background."

Next, identify the K lines from as many of the the known samples as possible and plot $\sqrt{V}$ vs. Z, where V is the voltage corresponding to the K_α peak. V is proportional to the energy of the X-ray.

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Symbol	Z
Cl	17
Ti	22
Cr	24
Fe	26
Ni	28
Cu	29
Zn	30
Ag	47
Cd	48
Sn	50
Gd	64
Ta	73
Au	79
Pb	82

Table 1: Table of known samples used in this lab. Note: The Cl source is in the form NaCl. Na ($Z = 11$) has too low of an energy to be measured with our equipment.

Determine the constants C' and σ, along with their fit uncertainties by a line fit to the equation

$$\sqrt{V} = C'(Z - \sigma) . \tag{3}$$

Then acquire X-ray spectra for the 6 unknown targets. Use your results above to make an initial determination of Z of each unknown target from the acquired spectrum and your $\sqrt{V}$ vs. Z trend.

Bohr's model predicts that the Rydberg constant is given by $R_\infty = me^4/4\pi c\hbar^3 = 1.0974 \times 10^7$ m^{-1}, where m and e are the mass and charge of the electron, respectively. The measured peak voltage V is proportional to the energy $E = hc/\lambda$ for a particular x-ray, but the proportionality constant depends on the detector design and its efficiency plus the operation of the detector electronics. To compare your measurements to Bohr's theory and R, you first need a conversion calibration. Use the known fact that for iron (Fe, $Z = 26$) the K$_{\alpha 1}$ x-ray has an energy of 6.403 keV to estimate a conversion constant between the measured voltage for the Fe K line and its known energy. Then apply this constant to your value for C' to compute the energy in keV of dominant x-rays from each of your samples. These values can be compared to the tabulated values accompanying this write-up.

Also calculate a value for C in the original form of Moseley's law, Eq. (2) from C'. How does this compare to that predicted by Bohr's equation, Eq. (1)?

Finally, Moseley's law is an approximation that works well for the K series of x-rays, but not so well for the L and other lines. In addition, there may be an offset in the conversion between the voltage and the energy of your detector: the use of a single point at 6.403 keV is not enough to establish a good calibration for your detector.

Thus, make a plot of known energies, from the look-up table, versus measured voltages. Fit this to a line so that you can convert any voltage to an energy (in keV). This is a "calibration curve" for your detector. Use this curve to convert the measured peaks of the unknowns to measured energies. From these numbers, check your initial determination of Z for the unknowns. Note: think about whether the peaks correspond to K lines or L lines. Also pay attention to what is reasonable, for example, your sample is unlikely to be a rare element (like plutonium) or a gas (like xenon)!

Extension Ideas

1. Acquire an X-ray spectrum for a number of the higher Z ($Z \geq 47$) elements and identify the L lines. Obtain the slope and intercept of $\sqrt{V}$ vs. Z as you did for the K lines. Interpret the values you derive for the slope and intercept, again in terms of the Rydberg constant R and σ, the number of electrons screening the nucleus for the L lines. Combine your estimated L-line energies to the tabulated values.

2. Take a much longer background run (1-2 hours or longer) and try to identify the X-rays in the background which are superimposed on any data you obtain with a given target. (Note: could some peaks come from the Co-57 source itself?)

3. Use your Moseley's Law to determine the primary elemental composition of samples of your choice.

4. Develop a multi-element sample with 3 to 4 strong peaks across the energy range that can be used to calibrate the energy scale in a single measurement.

3   Apparatus and Procedure

3.1   General Comments

This apparatus consists of a ^{57}Co radioactive source (same source as in the Mössbauer Experiment), a set of targets of different elements, and an Amptek XR-100CR semiconductor detector. This detector measures the X-ray energy directly, in contrast to Moseley's method of measuring X-ray wavelength. The advantage of a detector like ours is the compact size and ease of operation. However, for resolving closely spaced lines in an X-ray spectrum, wavelength measurement remains the standard.

The XR-100CR detector is optimized to detect photons in the energy range of 1 to 30 keV. The efficiency of the detector drops off rapidly at higher energies (see Fig 5). The output of the XR-100CR detector is conditioned and amplified, and then sent to a pulse height analyzer (PHA). This device plots number of counts on the y axis vs. voltage, in the form of channel number or voltage, on the x axis. A typical plot of the PHA output will look something like the plots in Figs. 2 and 4.

Caution: the radioactive source, target and detector are all located inside a lead lined box with a hinged lid. The lead lining provides sufficient shielding so that it is safe to be around the closed box for long periods of time. The source strength is sufficient that it is prudent to minimize the increased exposure when the lid is open. **Open the lid of the box only as necessary to change or remove targets. Be sure to keep the lid closed at all other times.**

3.2   The XR-100CR Detector

The XR-100CR semiconductor detector consists of a piece of silicon 300 μm thick. One side of the silicon (anode) is doped with an excess of p-type impurities, and the opposite side (cathode) with an excess of n-type impurities, resulting in the formation of a p-n junction, just as in a conventional diode. Within the silicon, electrons from the n-type region diffuse across the junction toward the p-type region, and holes from the p-type region diffuse across the junction toward the n-type region. This net migration of charge results in the development of a voltage across the p-n junction, and the
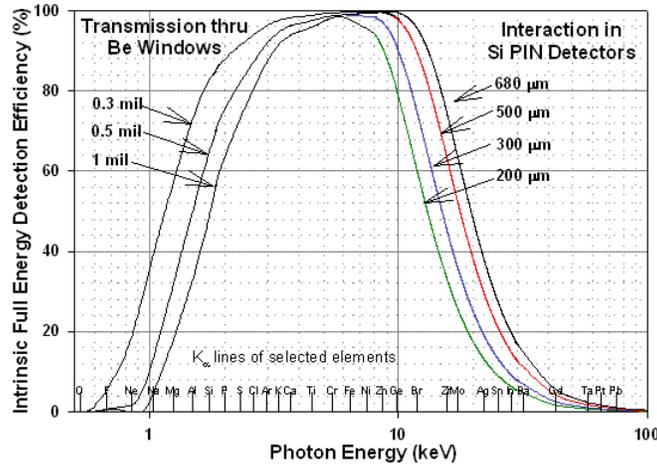
Figure 5: Efficiency curve of the Amptek XR-100CR

formation of a region in which there are no free charge carriers. This region is called the depletion region, and the electric field due to the charge migration reaches a maximum within this region. When electron-hole pairs are created in this region, the electric field acts to sweep the electrons and holes in opposite directions, resulting in a net current through the diode. Since the effect of incident radiation is to create electron-hole pairs in the silicon (one pair for every 3.62 eV of energy in the incident photon), the integral of the current pulse resulting from a photon impinging on the detector will be a measure of that photon's energy. The integral of the current pulse is in turn amplified to produce a shaped output pulse, the (peak) amplitude of which is proportional to the collected charge, and therefore incident photon energy.

The depletion region is clearly the key part of the detector, as electron-hole pairs formed there will move in opposite directions and contribute to the desired energy measurement. Increasing the width of this region increases the probability that the incident radiation will be stopped there and its energy deposited within the region. In order to increase the width of the depletion region, an external bias potential is applied across the detector, with the positive side connected to the cathode, and the negative side connected to the anode. (Note: this bias is applied in the opposite sense of a forward bias, and hence is termed a reverse bias.) The effect of the reverse bias is to pull electrons remaining in the n-type region and holes remaining in the p-type region even further from the p-n junction, resulting in a wider depletion region. In the absence of an external bias, the depletion region is typically some tens of μm wide, whereas with the bias applied, the depletion region can encompass almost the entire body of the silicon detector. The external bias also acts to increase the strength of the electric field in the depletion region, resulting in increased charge collection efficiency as electrons and holes are less likely to experience recombination or trapping when they are swept out of the region more rapidly.

Electron-hole pairs are also generated by thermal excitations in the silicon. Pairs so generated will add noise to energy measurements and degrade the resolution of the detector. In order to reduce the thermal generation of electron-hole pairs, the detector is cooled to approximately 250 K. The cooling is accomplished with a thermoelectric heat pump. The temperature is monitored by the attached meter, set to measure current. The current is calibrated to readout this kelvin temperature.

A natural question arises at this point: how linear is the XR-100CR detector? It turns out that

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semiconductor detectors are in general very linear, and the manufacturer of the XR-100CR quotes a linearity of 0.1% over the 1 to 30 keV design range of this device.

To protect the XR-100CR detector it is covered by a beryllium ($Z = 4$) window. To pass lower energy X-rays (several keV), this window must be very thin. The window on our detector is .001" thick. Such a thin window is, of course, very fragile, and being made of Be, also very brittle. **Any contact with the window can easily damage it.** In order to help protect the window, the red plastic cap (with a hole in the end) must be left in place at all times.

3.3 Procedure: preliminary setup

Now is a good time to turn on the XR-100CR amplifier/power supply if you have not already done so, along with the rest of the electronics (multimeter and oscilloscope). The power switch for the amplifier/power supply is at the back of the unit on the left side. The RTD (Rise Time Discriminator) should be on (switch up). Also turn on the DMM. The DMM current reading in amps indicates the detector temperature in kelvins. Typical operating current is 248 ± 2 μA.

The output pulses from the XR-100CR detector amplifier are positive-going, 0-8 volts peak amplitude. For a given energy incident photon, the amplitude of the output pulse will depend on the amplifier gain setting. The gain is set with the 10-turn potentiometer, and can be varied from 0 to 10.00 units (number in window is the integer, number on dial the fraction). Setting the gain involves a trade-off between the maximum energy you want to detect and the ability to resolve closely spaced lines. The lower the gain, the higher the energy you will be able to detect, but the energy scale will be more compressed and the more difficult it will be to resolve closely spaced lines. At maximum gain, the sensitivity is around 1 volt of output pulse amplitude per keV of incident photon energy. More precisely, with the gain set at 1.00, the detector creates pulses with heights of 1 volt per 8.4 keV of photon energy.

Before acquiring any spectra, choose an upper bound on the X-ray energy you wish to measure, and set the XR-100CR amplifier gain accordingly. Once this gain is set, it is a good idea to lock the 10-turn potentiometer with the small black lock lever to the right of the dial. As a practical matter, the highest Z target available in the lab that will yield a K spectrum in a reasonable amount of time is gadolinium, with Kα1 energy = 42.98 keV. With this number in mind, you also want to have a reasonable amount of "headroom", or signal above this maximum value so that you can resolve the highest energy. A good choice is to use 50 keV as a rough maximum energy, and to set the gain so that you get peak heights of about 7.5 volts with this energy. To record a 50 keV photon so that it has a pulse height of about 7.5 volts, a proportional argument gives

$$\frac{\text{Gain} = 1.0}{1 \text{ V}/8.4 \text{ keV}} = \frac{\text{Gain} = x}{7.5 \text{ V}/50 \text{ keV}} \rightarrow x \approx 1.26 \tag{4}$$

Try setting the gain there (or, if it is already at this setting, leave it there) and adjust as necessary. Note that to convert accurately from voltage to energy, you cannot rely on the gain setting. You will need to calibrate the energy scale using the tabulated emission energies of the known samples. Such a calibration should be repeated at the start of each recording session and any time the gain knob is adjusted.

The amplifier output is connected to the input of a computer-based high speed data acquisition card. A LabVIEW application is used to perform the data acquisition and create a pulse-height histogram from the input pulse waveforms. The user of the program may select the resolution of

the histogram, i.e., the number of bins, along with other parameters. The resulting data sets can also be analyzed to find peak locations and widths in terms of the pulse height voltages.

Start the LabVIEW application according to the instructions from the TA or lab manager. A variety of parameter choices will produce a reasonable spectrum, but experience shows that the settings in Table 2 are a good place to start.

Parameter	Value
Low level disc	about 300 mV
Digitizer run time	0
Digitizer input	Ch 1
Digitizer vertical range	10 V
Digitizer sample rate	20.00 MHz
Digitizer record length	(ignore*)
Digitizer mode	Continuous
Histogram update	5 cycles
Histogram bins	800
Histogram minimum	0 V
Histogram maximum	7.9 to 8.0 V*

Table 2: Starting values for data acquisition parameters. *In continuous mode, the record length defaults to the maximum available. If too many counts show up at the 8 volt max, back the histogram maximum off a bit to 7.9 V.

3.4   Acquiring a Spectrum

Before placing any targets in the lead lined box, the TA, Professor or lab manager will go over the hardware arrangement inside the box with you. Again, it is prudent to minimize the time that the lid is open so as to minimize radiation exposure. After going over the hardware arrangement inside the box, place a target (Fe is a good one to start with) in the holder and close the lid.

Start the LabVIEW application "Pulse Height Analyzer" whose icon should be on the desktop. When it starts, the program will load the most recent data set. Set the parameters as suggested in Table 2. Before collecting data, clear any old data by clicking on the CLEAR button. Then start data acquisition by clicking on the TAKE DATA button. After a short delay you should see the blue dots of the histogram graph appear. Let the data taking run until you can see clear peaks appear, and then a bit more until the spectrum is well established; aim for at least 100 counts in the peaks you want to analyze. Record the duration of the run. (Note: with the "run time" set to "0", the analyzer will run until you hit the Stop button. To collect data for a preset length of time, enter any nonzero run time.)

After you stop the data acquisition (how should be obvious), it is a good idea to save the data set with the SAVE DATA button and to print out the entire spectrum with the PRINT DATA button. Then you can use the ANALYZE DATA dialog box to fit a Gaussian peak shape to the important peaks. Detailed instructions for using the pulse height analyzer and analysis feature are available under the SHOW INSTRUCTIONS buttons.

3.5   Some hints on data collection and analysis

- Your goal is to measure the characteristic peaks associated with each sample. Start with iron (Fe) to get a strong K_α peak at about 1 volt (assuming the recommended settings). Then collect data for samples by moving away from Fe in terms of Z both higher and lower.

- For each successive run, pay attention to the new peaks. If you identify the characteristic lines of one sample, you should be able to estimate the location of the peaks you should get with others.

- Think about which peaks in a given spectrum are worth fitting. Don't waste time fitting background peaks (unless you are actually analyzing the background.) The best way to choose is to pay attention to what is new in each spectrum.

- The K line may or may not be the strongest peak in a run, depending on the sample. Some samples will show only K lines, some only L lines, and some both.

- The uncertainty calculated by the fitting program is NOT the uncertainty in your experiment. It is only the uncertainty for that particular fit of that particular set of data. A better measure of the uncertainty is to make a number of measurements of the same sample, fit each one, and then analyze the distribution of fit results.

- The overall time of data collection does not matter. What matters is the quality of the statistics for a particular spectrum. If the counting efficiency is low, count longer.

References

[1] R. Eisberg and R. Resnick, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2nd ed., Wiley, New York, 1985, p. 342.

[2] H. Haken and H. Wolf, The Physics of Atoms and Quanta, Springer, New York, 1996, pp. 314.

Prepared by J. Stoltenberg, R. Van Dyck, D. Pengra, and J. A. Detwiler
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