X-ray Scattering

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Abstract

X-ray scattering techniques are a family of non-destructive analytical techniques which reveal information about the crystal structure, chemical composition, and physical properties of materials and thin films. X-ray scattering has important applications including the discovery of the double-helix structure of the DNA. In this experiment, we obtained the x-ray spectra to find Planck's constant using a molybdenum target as an x-ray source. We found Planck's constant as $4.2 \pm 1.5 \times 10^{-34}$. Our result is two sigma away from the real value; however, considering our sigma result is big, still, our result is not that much convincing.

1 Theoretical Motivation

X-rays originate from atomic electrons and from free electrons decelerating in the vicinity of atoms. Radiation-producing devices produce X-rays by accelerating electrons through an electrical voltage potential and stopping them in a target. Many devices that use a high voltage and a source of electrons produce X-rays as an unwanted byproduct of device operation. These are called incidental X-rays. Most X-ray devices emit electrons from a cathode, accelerate them with a voltage, and allow them to hit an anode, which emits X-ray photons. These X-ray photons can be categorized as Bremsstrahlung or Characteristic. When electrons hit the anode, they decelerate or brake and emit Bremsstrahlung (Figure 1)². Bremsstrahlung is produced most effectively when small charged particles interact with large atoms, such as when electrons hit a tungsten anode. However, Bremsstrahlung can be produced with any charged particles and any target. For example, at research laboratories, Bremsstrahlung has been produced by accelerating protons and allowing them to hit hydrogen. When electrons change from one atomic orbit to another, characteristic X-rays are produced. The individual photon energies are characteristic of the type of atom and can be used to identify very small quantities of a particular element. For this reason, they are important in analytical X-ray applications at research laboratories.³

¹https://en.wikipedia.org/wiki/X-ray_scattering_techniques

²Figure 1 is taken from https://en.wikipedia.org/wiki/Bremsstrahlung#/media/File:Bremsstrahlung.svg

³https://www.wku.edu/ehs/radiation/module-9_production_of_x-rays.pdf "Production of X-rays, Radiation Safety Training for Analytical X-Ray Devices, Western Kentucky University"

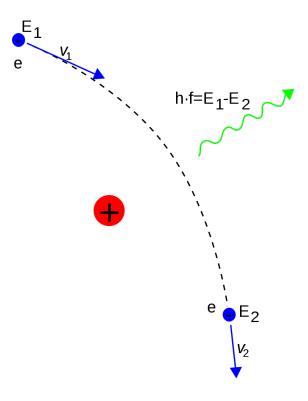


Figure 1: Bremsstrahlung

Solids having crystal structures are very convenient as a target to observe interference since we know the seperation between the molecules. When two photons are incident on molecules at two consecutive layer of a crystal structure, they are reflected with the same angle with the incident angle. (See Figure 1) However, there is a $2dsin\theta$ path difference between these two rays where d is the distance between two molecule of our crytal. The Bragg's law states that the x-rays scattered from a crystal will form maxima at the angles satisfying the following equation.

$$2dsin\theta = m\lambda \tag{1}$$

where m is some integer called the order of the diffraction maxima and λ is the wavelength.

In the paper which William Duane and Franklin Hunt published in 1915, they stated that their results show that the minimum voltage V_0 required to produce X-rays of λ_0 is given by the energy equation

$$V_0 e = h\nu_0 = \frac{hc}{\lambda_0} \tag{2}$$

where e = electron charge, c = velocity of light, and also the energy radiated per second at this wave-length λ_0 is infinitely small.⁴

⁴https://journals.aps.org/pr/pdf/10.1103/PhysRev.6.166 "On X-ray Wave-lengths by William Duane and Franklin L. Hunt", The American Physical Society, 1915

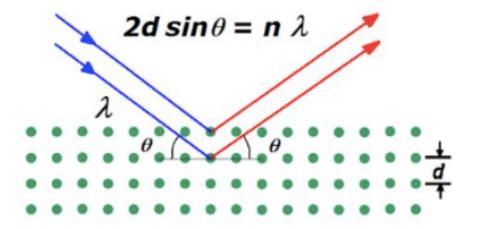


Figure 2: Two photons which are reflected from a crystal surface

In the analysis, we took speed of light to be equal to 299 792 458 meters per second. The separation between NaCl molecules which we used as target for scattering was d=282 pm. For the wavelenghts of K-level emission lines of the Molybdenum, we used the wikipedia values as $K_{\alpha 1}=0.0709$ nm and $K_{\beta 1}=0.0632$ nm. ⁵

Throughout the analysis we propagated error as follows.

$$\sigma = \sqrt{\sum_{i} \left(\frac{\partial f}{\partial n_i}\right)^2 \sigma_i^2} \tag{3}$$

2 Apparatus and Procedure

In the experiment, we used X-ray tube with Molybdenum source, PHYWE X-ray unit, Geiger counter, NaCl Crystal, and a computer.

Our X-ray tube was producing X-rays both by Bremsstrahlung and by the deexcitation of electrons. The details of the both mechanisms are given in the Theoretical Motivation part. After generating the X-rays, we send them to the NaCl crystal target to observe interference according to Bragg's law (see Equation 1) The experiment consists two parts. In the first part, we did calibration with use of the K-lines of the spectra we got. To do this, we first set the type of the data as spectra and arranged the voltage to the constant 35 kV. This voltage was used to speed up electrons which hit to the Molybdenum. We set the x-data as crystal angle. We arranged crystal angle so that it starts at 3 degrees and end at 45 degrees with 0.1 increments. Detector angle was twice the crystal angle throughout the experiment. We set our emissions current to 0.8 mA and integration time as 5s. We used no absorber and no filter. We chose all at the Displays section. Then, for the second part, we just changed the voltage to the 15kV and stopping angle to 20 degrees. We stopped taking data when we see the plateau. We repeated same procedure up to 30 kV by incrementing

⁵https://en.wikipedia.org/wiki/X-ray



Figure 3: General view of apparatus

voltage by 3kV each time. The computer gave us the number of counts corresponding to each crystal angle.

3 Data and Analysis

The graph of the data taken at first part is given below. 6

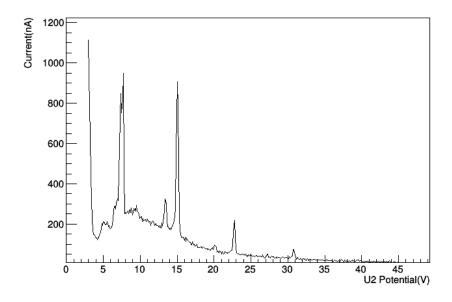
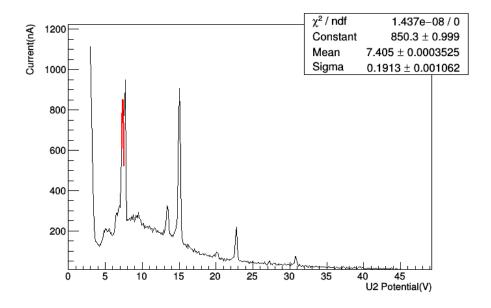
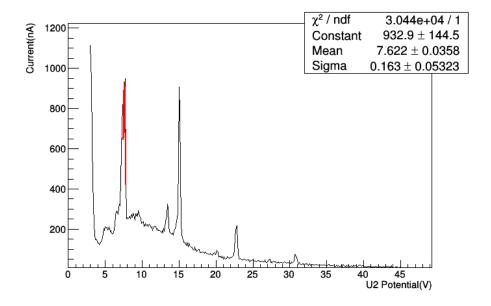


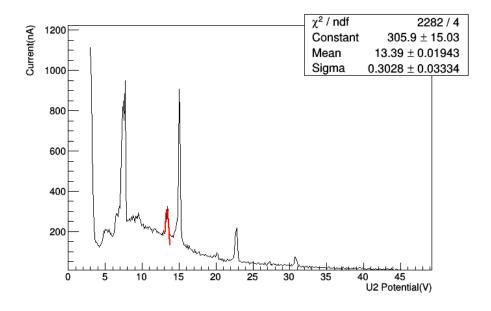
Figure 4: The graph corresponding to 35 kV

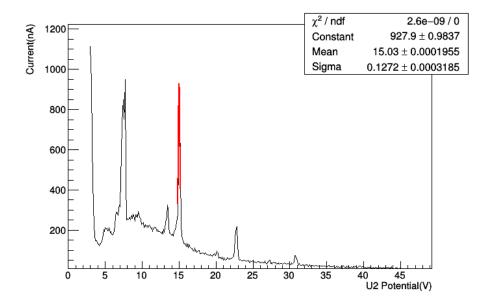
 $^{^6}$ The graphs of first part (calibration part) has wrong axes labels. X-axis supposed to be labeled as crystal angle (degrees) and y-axis should be labeled as accumulation rate.(Imp/s)

We did Gaussian fits to each K_{alpha} and K_{beta} line as follows.

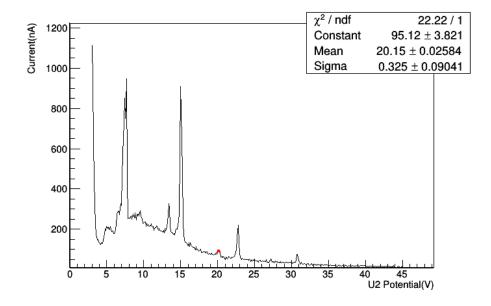


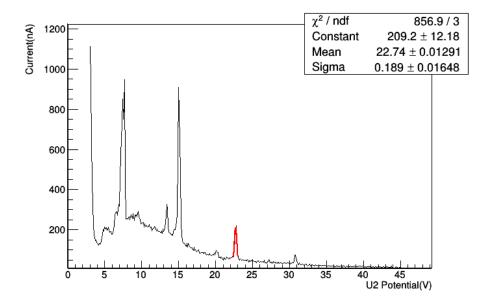




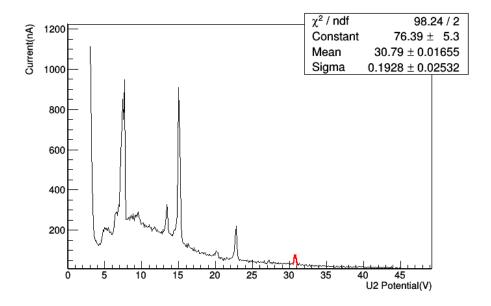


The K_{β} line for m = 4 is invisible in noise.





The mean values of that Gaussian fits gave us the angle corresponding to peak values. We round these numbers off to the one digit after decimal point since our increment angle was 0.1 degree.



Then we also calculated the theoretical theta values by Bragg's law for each m using the wavelength values given at the end of Theoretical Motivation part.

The theoretical values are found as follows in degrees:

$$\theta_{\beta 1} = 6.4$$
 $\theta_{\alpha 1} = 7.2$
 $\theta_{\beta 2} = 12.0$
 $\theta_{\alpha 2} = 14.6$
 $\theta_{\beta 3} = 19.6$
 $\theta_{\alpha 3} = 22.2$
 $\theta_{\alpha 4} = 30.2$

Here, the convention for notation is such that, for example, $\theta_{\alpha 1}$ represents the the angle corresponds to the line K_{α} for m = 1.

Then, we plotted the graph of experimental versus theoretical thetas.⁷ (see Figure 12) This graph was used for calibration so that

 $1.0 \pm 0.0 \times (thetaexperimental) + (-0.61 \pm 0.10) = (thetatheoretical)$

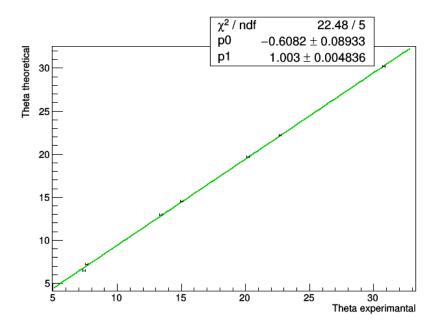


Figure 12: Calibration graph

The graphs for the data taken in the second part are given below. We fit a line to a small portion of the rise of the counts resulting from Bremsstrahlung to find θ_{min} . We searched for θ_{min} because we want to use Duane-Hunt law to relate voltage to frequency, and for that relation to hold, the electron's full energy must create a single atom. This requires max frequency, and consequently, min wavelength, which corresponds to min theta by Bragg's law.

⁷p0 is slope while p1 is y intercept.

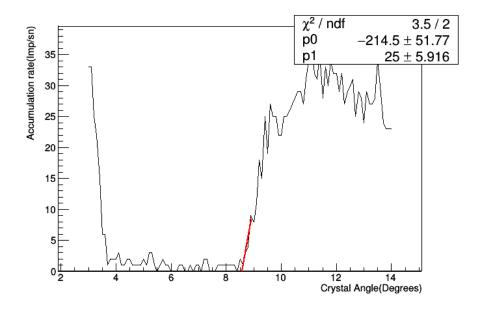


Figure 13: The graph corresponding to 15 kV

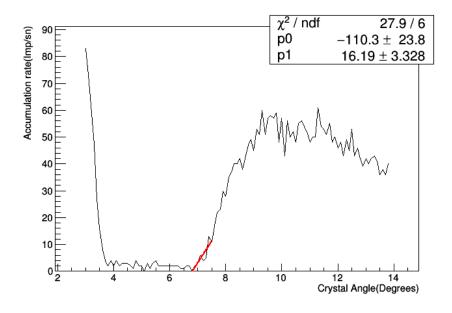


Figure 14: The graph corresponding to 18 kV

After finding θ_{min} values by the slope and y-intercept of the graphs, we corrected them using our calibration relation.⁸ After, we got the corresponding frequency values using Bragg's law. Then, we plotted the frequency versus electron-volt(corresponding voltage values times electron's charge) graph.⁹(Figure 19)

⁸The calculations of θ_{min} values, corrected θ_{min} values and the all calculations till end of the analysis as well as uncertainty calculations can be found in the spreadsheet in the link given at Appendix.

⁹The label of the y-axis must be corrected as Energy(eV). Here, slope is p1.

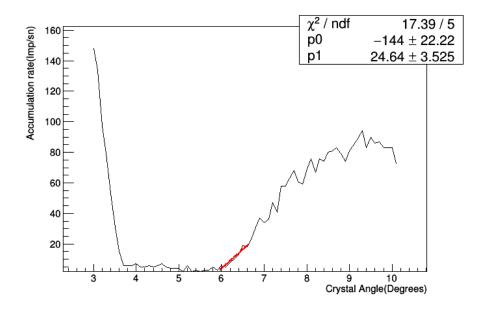


Figure 15: The graph corresponding to $21~\mathrm{kV}$

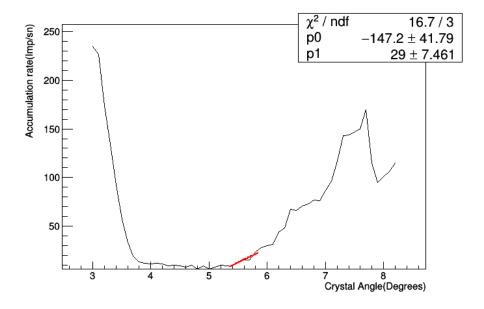


Figure 16: The graph corresponding to 24 kV

The slope of the graph given at Figure 19 is Planck's constant by Equation 2. Thus, we found

$$h = 4.2 \pm 1.5 \times 10^{-34} Js \tag{4}$$

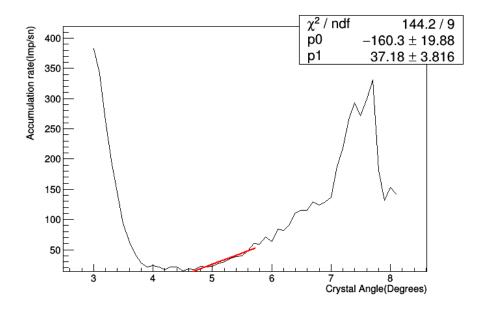


Figure 17: The graph corresponding to 27 kV

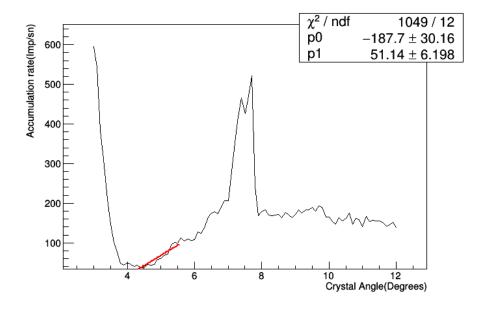


Figure 18: The graph corresponding to 30 kV

4 Conclusion

Our result is two sigma away from the accepted value. It is not bad in first sight however our sigma value is a bit big. Unfortunately, there was almost nothing to do about it since the uncertainty arises from the uncertainty values of the minimum angles which we found from the data we read at fit panel.

We performed the calibration in first part to see how our setup's data deviate from the

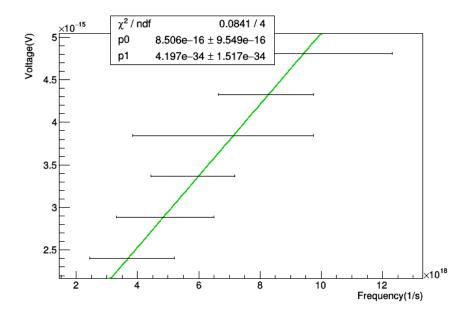


Figure 19: Frequency versus voltage graph

real values. This was good for decrease the error resulting from the setup.

The jumps in our graphs at around 5 degree or lower is because at the beginning since the angle is zero and there is no scattering at all, the x-rays were trivially counted by counter. After the angle arises a bit, the counts decreases as expected since scattering starts.

We see only K-lines because the order of the energy is only enough for the K-lines, not L-lines or so on.

There is a non-zero intercept in our final graph (Figure 19) which is an unexpected phenomena. It is because of the errors such as the counts resulting from maybe the background radiation and which are counted even there are no x-rays produced by us.

5 Appendix

References are given as footnotes. The codes used in analysis and also the spreadsheet file in which the calculations are done can be found in the following github link:

https://github.com/beratgonultas/phys442/tree/master/xray