XRD Experiments

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First Lab Report for PHYS403

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Abstract

This document reports on three X-Ray Diffractions (XRD) experiments: (i) Fine structure of the characteristic x-radiation of a molybdenum anode. (ii) *Duane-Hunt* relation and determination of *Plank*'s constant. (iii) *Bragg reflection*: diffraction of x-rays at a mono-crystal.

1 Fine structure of the characteristic x-radiation of a molybdenum anode.

1.1 Introduction

When radiation with a wavelength comparable to atomic spacing is scattered in a fashion like a mirror, by the atoms of a crystalline system, it undergoes constructive interference and causes Bragg diffraction. In a crystalline solid, the waves are scattered from lattice planes that are $\boldsymbol{d}$ layers apart from one another:

$$n\lambda = 2d\sin\theta$$

Where λ is the wavelength of x-rays, n is the order of diffraction, d is the lattice (atomic) spacing, and θ is the angle of incidence.
In this experiment, we will investigate the characteristic x-rays that comes out from a molybdenum target. Then, we will try to split the doublets of K_α & K_β by applying higher order of diffraction.

1.2 Experimental Setup

In this experiment, we will use an $NaCl$ crystal with a known lattice spacing $d = 282.01\ pm$ and we will detect its characteristic x-rays. Using this setup:

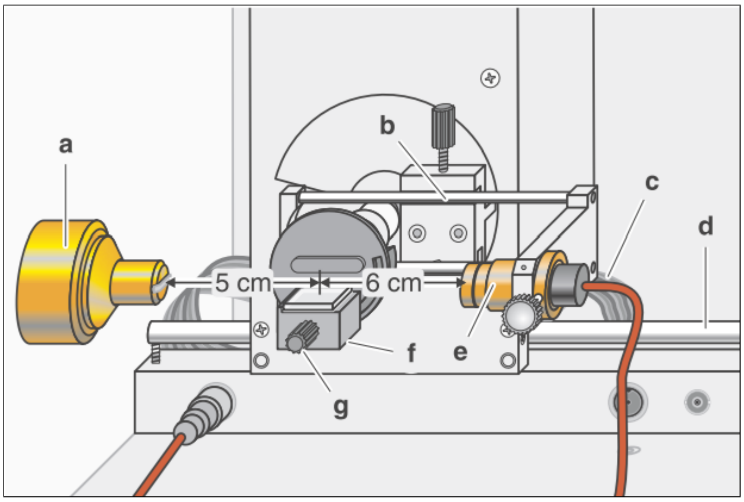

Figure 1: X-ray machine setup

The x-ray beam will come out from **a**, then it will get collimated, then it will scatter out of the crystal, and finally detected at **e**.

1.3 Results & Discussion

1.3.1 First Order Diffraction

For this part, we set the tube accelerating voltage $U = 35\ kV$, with tube current $I = 1.00\ mA$ and the angle was ranging from $5.5° \ to\ 8.0°$ with $\Delta\beta = 0.1°$, and $\Delta t = 10\ s$

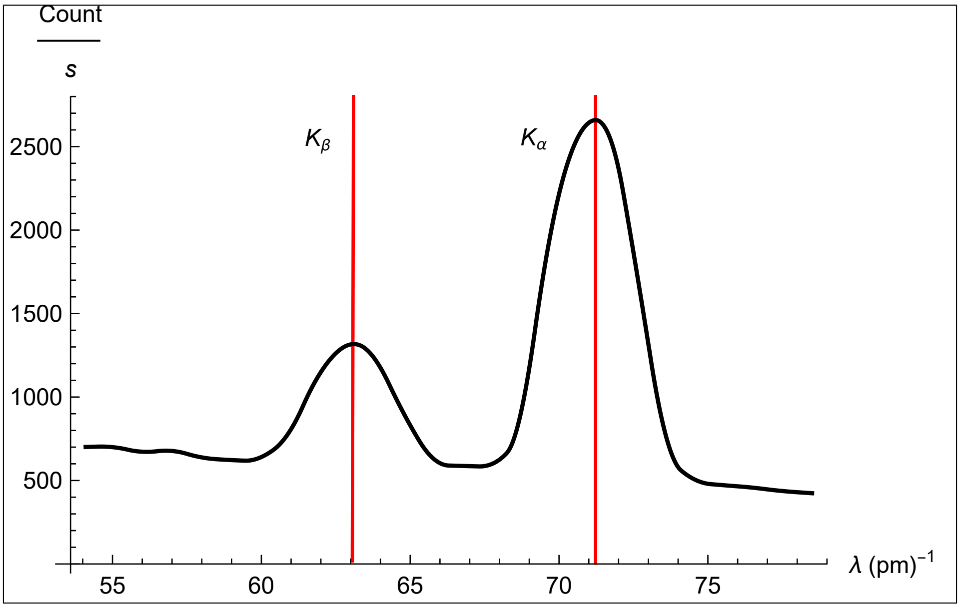

Figure 2: Characteristic x-ray K_α and K_β

We can see that the peaks at K_α and K_β are wide, which could indicate that there is more than one line in there, we shall uncover that using a higher order of diffraction, the fifth.

Line Doublet	Measured Results ($\frac{\lambda}{pm}$)	Literature Results ($\frac{\lambda}{pm}$)	%Error
K_α	70.7	71.08	0.54%
$K_\beta + K_\gamma$	62.9	63.09	0.30%

Table 1: Results for the first part

1.3.2 Fifth Order Diffraction

In this part, we changed the interval of the angles, to range from $32.5° \ to\ 40.5°$, and $\Delta t = 720\ s$. After collecting counts for 16 hours, we obtained this plot:

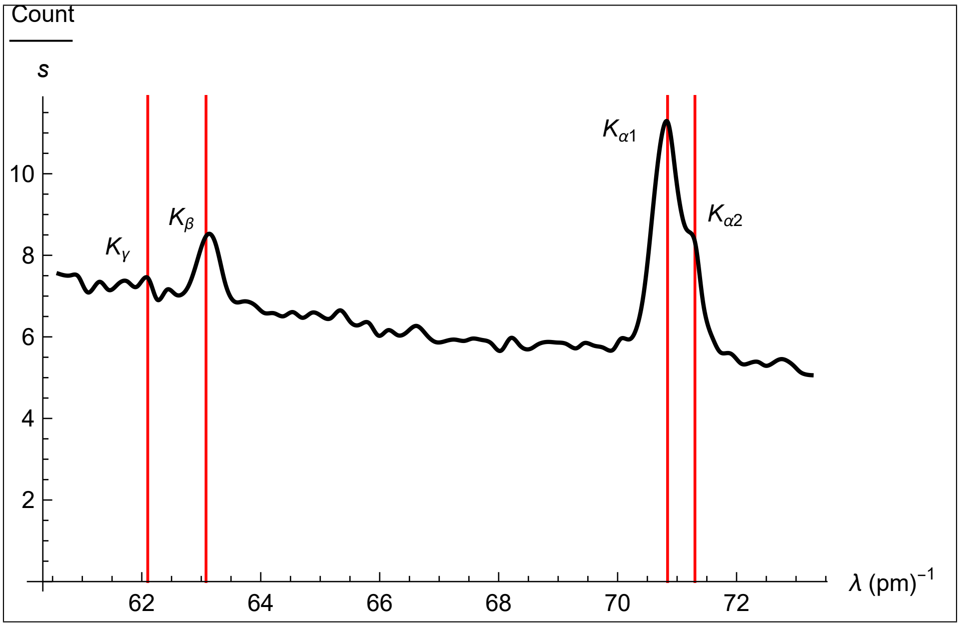

Figure 3: Characteristic x-ray K_α split into $K_{\alpha 1}$ & $K_{\alpha 2}$ and K_β into K_β & K_γ

We can notice that the line doublets in the first part was split and can be observed individually.

Lines	Measured Results ($\frac{\lambda}{pm}$)	Literature Results ($\frac{\lambda}{pm}$)	%Error
$K_{\alpha 1}$	70.84	70.93	0.63%
$K_{\alpha 2}$	71.30	71.36	0.08%
K_β	63.08	63.26	0.28%
K_γ	62.1	62.09	0.02%

Table 2: Results for the second part

Splitting of doublet K_α: $\Delta\lambda = 0.3\ pm$, which is 7.0% away from literature.

Splitting of doublet $K_{\beta 1}$ & K_γ: $\Delta\lambda = 1.17\ pm$, which is 16.2% away from literature.

1.4 Conclusion

We can see that we remove the splitting of the doubles by using the fifth order of diffraction. The results we obtained were very close to literature.

2 *Duane-Hunt* relation and determination of *Plank*'s constant.

2.1 Introduction

The *Duane-Hunt* relation shows the inverse proportionality between the minimum x-ray wavelength of the bremsstrahlung continuum in the emission spectrum of an x-ray and the tube voltage:

$$\lambda_{min} \propto \frac{1}{U}$$

Knowing that the minimum wavelength occurs at the highest frequency, and the highest frequency is associated to the energy by:

$$E_{max} = h\nu_{max}$$

Knowing that the maximum energy happens at the moment in which it acquires the total kinetic energy of an electrode decelerated in the anode:

$$E = e \cdot U$$

Then, we can conclude that:

$$h\nu_{max} = e \cdot U \implies \lambda_{min} = \frac{hc}{e}\frac{1}{U}$$

Thus, if we have a function of λ_{min} $vs.$ $\frac{1}{U}$ Then the slope is going to lead us to Planck's constant.

2.2 Results & Discussion

2.2.1 Confirming The *Duane-Hunt* Relation

We can confirm their relation by varying the accelerating voltage and plotting the radiation profile:

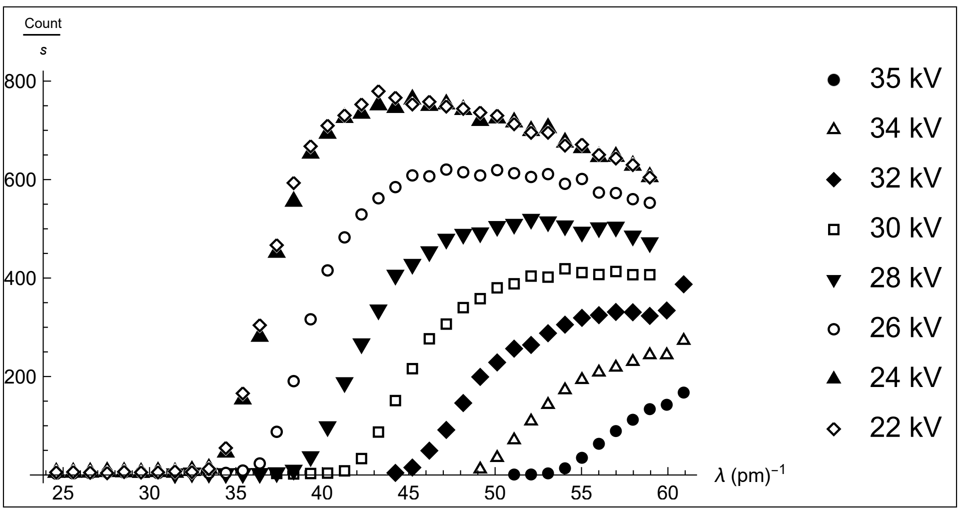

Figure 4: Counts vs. wavelength for different accelerating voltage

As we can see, the higher the accelerating voltage the lower the value of λ_{min}. Which means the relation is confirmed.

2.2.2 Calculating Planck's Constant

Now, we will plot the best line fit for the values of λ_{min} across all inverses of the accelerating voltage:

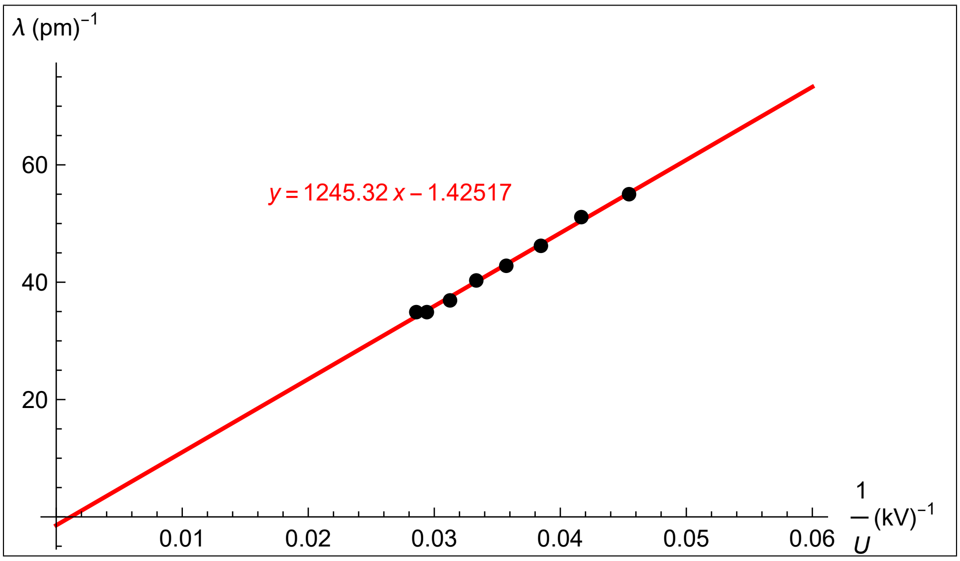

Figure 5: λ_{min} $vs.$ $\frac{1}{U}$ for all the accelerating voltages

The slope of the best line fit is related to Planck's constant by:

$$Slope = \frac{hc}{e} \implies h = \frac{1.6022 \times 10^{-19} \times (1245.32 \pm 32.5748 \times 10^{-9})}{299792458} = 6.655 \pm 0.17 \times 10^{-34}$$

$$\%Error = \left| \frac{6.655 \times 10^{-34} - 6.626 \times 10^{-34}}{6.626 \times 10^{-34}} \right| \times 100 = 0.44\%$$

2.3 Conclusion

We were able to confirm the *Duane-Hunt* relation, by varying the accelerating voltage, and then observing the shift of the minimum wavelength that was caused by the increase of the accelerating voltage. Then, we determined Planck's constant by fitting the minimum wavelength linearly, and found that it lies within the literature value!

3 *Bragg Reflection*: Diffraction of x-rays at a Mono-crystal.

3.1 Introduction

In this experiment, we will attempt to confirm Bragg law, which we have used in **Section 1**.

$$n\lambda = 2d \sin\theta$$

In order to do this, we will scan wide range of scattering angles off a $NaCl$ crystal with a known lattice spacing $d = 282.01\ pm$, starting from $2.0°\ to\ 25°$, with accelerating voltage $U = 35\ kV$, and tube current $I = 1.00\ mA$, and $\Delta t = 10\ s$.

By doing so, we will encounter multiple orders of diffraction, specifically three. By using Bragg's law, we will be able to confirm whether the angles correspond to the right wavelength of characteristic x-rays K_α & K_β.

3.2 Results & Discussion

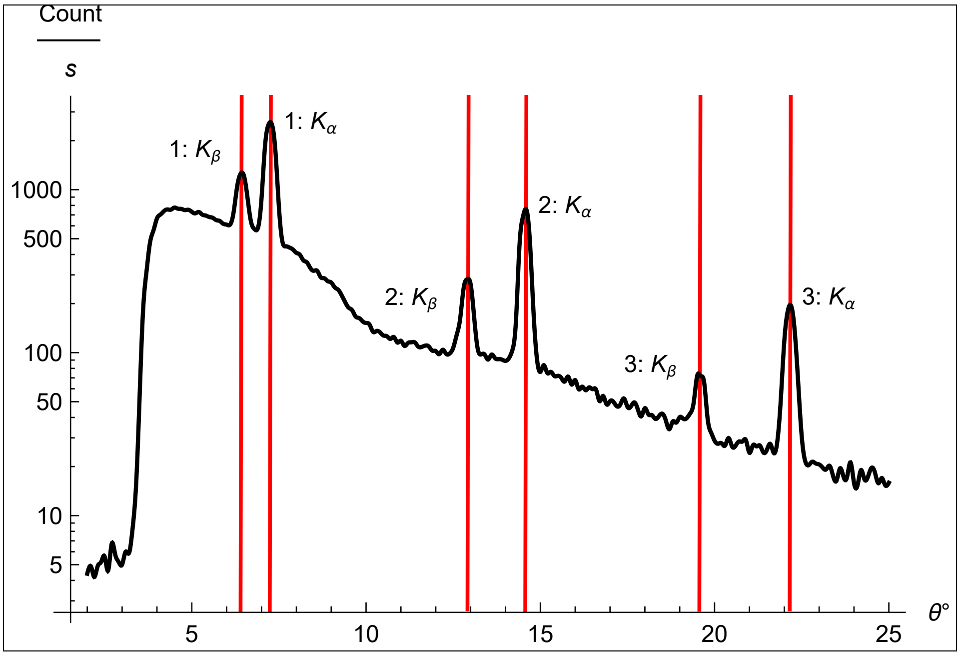

Figure 6: Log scale for $\lambda\ vs.\ counts$

As we can see, we obtained three different orders of diffraction. we can use Bragg's law to determine the correspondent wavelength:

n	$\theta(K_\alpha)$	$\frac{\lambda}{pm}(K_\alpha)$
1	7.3°	71.67
2	14.6°	71.09
3	22.3°	71.34

Table 3: K_α lines obtained from Bragg's law

n	$\theta(K_\beta)$	$\frac{\lambda}{pm}(K_\beta)$
1	6.4°	62.87
2	12.9°	62.96
3	19.6°	63.07

Table 4: K_β lines obtained from Bragg's law

	$\frac{\lambda}{pm}(K_\alpha)$	$\frac{\lambda}{pm}(K_\beta)$
Mean Value	71.37	62.97
Literature Value	71.08	63.09
%Error	0.41%	0.20%

Table 5: Comparing obtained results to literature

3.3 Conclusion

In this experiment, we were able to confirm Bragg's law by obtaining three orders of diffraction of an $NaCl$ monocrystal. Then, we compared the characteristic wavelengths of K_α & K_β to the literature, and obtained a small percentage error.

4 Three Experiments' Conclusion

These three XRD experiments were done on a x-ray generating machine with molybdenum target. We were able to conduct these experiments with small margins of errors. The main law that was used was Bragg's law.