

Analysing the intensity of the copper X-radiation as a function of the Bragg angle

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Abstract

This experiment investigated the characteristic X-ray emission spectrum of a copper anode using Bragg diffraction. X-radiation was diffracted by an analyzing crystal with an assumed interplanar spacing of $d = 1.36 \text{ \AA}$, and the radiation intensity was measured as a function of the Bragg angle, θ . Two distinct intensity peaks were observed at angles of $\theta_1 = 34.7^\circ$ and $\theta_2 = 38.5^\circ$. Using Bragg's Law, the energy corresponding to the first peak was calculated to be 8.010 keV . This result is in excellent agreement with the accepted literature value for the copper $K\alpha$ transition (8.048 keV), yielding a relative error of only -0.47% . The experiment, therefore, succeeded in obtaining a high-precision value for the $K\alpha$ and $K\beta$ energy.

1 Introduction

X-rays, a form of high-energy electromagnetic radiation, have been a pivotal tool in science since their discovery, allowing for the direct investigation of crystalline structures and atomic-level phenomena. The generation of X-rays for such analysis is commonly achieved in an X-ray tube, where a metallic anode, in this case copper, is bombarded with a beam of high-energy electrons. This interaction produces two distinct types of X-ray spectra: a continuous spectrum known as Bremsstrahlung (or "braking radiation"), which results from the deceleration of electrons as they interact with the atoms of the target, and a discrete spectrum of characteristic X-rays, which are unique to the anode material (PHYWE, n.d.-a). This characteristic radiation arises when an incident electron ejects an inner-shell electron from a target atom. The subsequent de-excitation, as an electron from a higher energy level fills the vacancy, results in the emission of an X-ray photon with an energy corresponding to the difference between the two atomic energy levels.

The characteristic emission spectrum of copper is dominated by two prominent peaks known as the K_α and K_β lines, which correspond to electron transitions from the L and M shells, respectively, into a vacancy in the innermost K shell (Tel-Aviv University, n.d.). While appearing as single peaks at low resolution, these lines possess a complex fine structure that has been the subject of extensive theoretical and experimental investigation (Deutsch et al., 1995; Chantler et al., 2009). To analyze the wavelengths of these characteristic X-rays, the principle of Bragg diffraction is employed. When a polychromatic X-ray beam is incident upon a single crystal, constructive interference occurs only at specific angles where Bragg's Law is satisfied:

$$n\lambda = 2d\sin\theta \quad (1)$$

Here, n is an integer representing the order of diffraction, λ is the wavelength of the X-ray, d is the interplanar spacing of the analyzing crystal, and θ is the glancing angle of incidence, also known as the Bragg angle. At angles that satisfy this condition, the reflected waves are in phase, producing a peak in measured intensity.

The objective of this experiment is to analyze the intensity of X-radiation produced by a copper anode as a function of the Bragg angle, θ . By directing the X-ray beam onto a Potassium Bromide (KBr) monocrystal and measuring the resulting radiation intensity at varying angles, the characteristic K_α and

K_β emission lines can be identified as distinct peaks above the Bremsstrahlung background. From the angular positions of these peaks for various orders of diffraction (n), the wavelengths and corresponding energies of the characteristic copper X-rays will be determined and compared with established values (PHYWE, n.d.-b). This investigation serves as an experimental verification of the quantum nature of atomic energy levels and demonstrates the powerful application of Bragg's Law in X-ray spectroscopy.

2 Theory

The experimental analysis of characteristic X-rays relies on two fundamental physical processes: the generation of X-rays within an X-ray tube and their subsequent diffraction by a crystalline structure. This section outlines the theoretical principles governing these processes. When high-energy electrons, accelerated by a large potential difference, strike a metallic target such as a copper anode, their kinetic energy is converted into electromagnetic radiation through two primary mechanisms. As the incident electrons pass through the copper target, they are deflected and decelerated by the strong electric fields of the copper nuclei. According to classical electromagnetic theory, any accelerating or decelerating charge radiates energy. This process, termed Bremsstrahlung (German for "braking radiation"), produces a continuous spectrum of X-rays. The energy of the emitted photons can range from zero up to the maximum kinetic energy of the incident electrons. The minimum possible wavelength, λ_{\min} , corresponds to an electron losing all of its kinetic energy in a single collision and is given by the Duane-Hunt Law:

$$\lambda_{\min} = \frac{hc}{eV} \quad (2)$$

where h is Planck's constant (6.626×10^{-34} J · s), c is the speed of light (3.0×10^8 m/s), e is the elementary charge (1.602×10^{-19} C), and V is the accelerating voltage applied to the X-ray tube. This equation defines the sharp cutoff on the short-wavelength end of the X-ray spectrum.

Superimposed on the continuous Bremsstrahlung spectrum are sharp, high-intensity peaks known as characteristic X-rays. These arise from atomic-level quantum transitions within the target atoms (Tel-Aviv University, n.d.). If an incident electron has sufficient energy, it can eject an electron from one of the inner atomic shells (e.g., the K shell, $n=1$). This leaves a vacancy in the shell, putting the atom in a highly excited and unstable state. To return to a lower energy state, an electron from a higher energy shell (e.g., the L shell, $n=2$, or M shell, $n=3$) transitions "down" to fill the vacancy. The excess energy is released as an X-ray photon with a precisely defined energy equal to the difference between the initial and final energy levels of the transitioning electron.

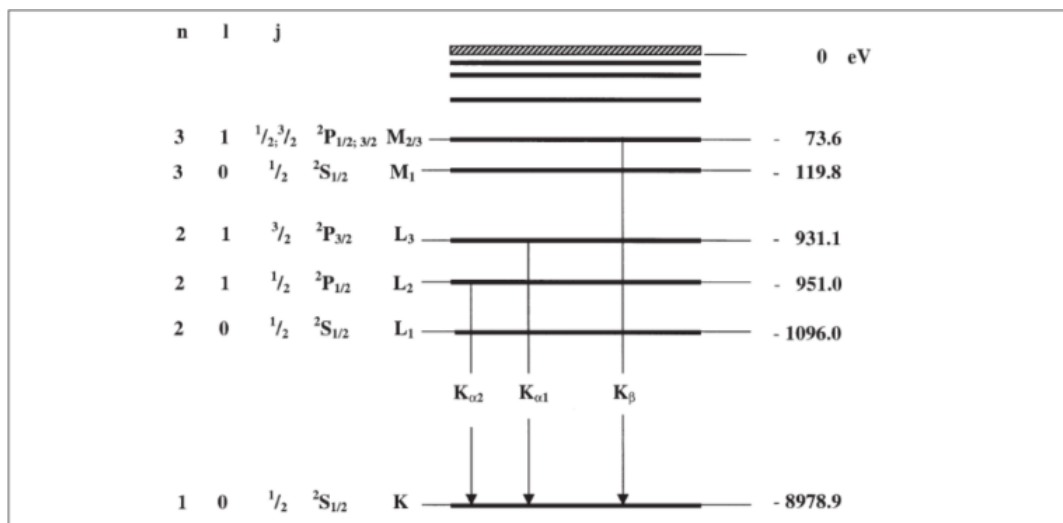


Figure 1

The resulting emission spectrum is characteristic of the anode material. For copper, the most prominent lines are:

- **K_α line:** An electron from the L shell ($n=2$) transitions to the K shell ($n=1$). This is the most intense line.
- **K_β line:** An electron from the M shell ($n=3$) transitions to the K shell ($n=1$). This line is of higher energy (shorter wavelength) but lower intensity than the K_α line.

The wavelengths of these characteristic lines for a given element are described by Moseley's Law, which relates the wavelength to the atomic number (Z) of the target material:

$$\frac{1}{\lambda} = R_\infty (Z - \sigma)^2 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \quad (3)$$

where R_∞ is the Rydberg constant, σ is a screening constant, and n_i and n_f are the principal quantum numbers of the initial and final electron states. This relationship confirms that the emission spectrum is a unique fingerprint of the element. Advanced studies show these lines have a fine structure (e.g., the K_α line is a doublet of $K_{\alpha 1}$ and $K_{\alpha 2}$), which arises from relativistic and electron-electron interaction effects (Deutsch et al., 1995).

To measure the wavelengths of the characteristic X-rays, they are directed onto a single crystal with a known, regular atomic structure. The layers of atoms in the crystal act as a natural three-dimensional diffraction grating. Constructive interference of the scattered X-rays occurs only when the path difference between waves reflecting off adjacent atomic planes is an integer multiple of the wavelength. This condition is described by Bragg's Law (PHYWE, n.d.-a):

$$n\lambda = 2d \sin \theta \quad (4)$$

Here, n is an integer (1, 2, 3, ...) known as the order of diffraction, λ is the X-ray wavelength, d is the interplanar spacing of the crystal, and θ is the glancing angle at which constructive interference is observed. For the Potassium Bromide (KBr) crystal used in this experiment, the interplanar spacing for the (100) plane is $d = 329$ pm. By measuring the angles θ at which intensity peaks are found, and knowing d and the order n , the wavelength λ can be calculated.

Once the wavelengths of the characteristic K_α and K_β lines are determined using Bragg's Law (Eq. 4), their corresponding photon energies (E) can be calculated using the Planck-Einstein relation:

$$E = \frac{hc}{\lambda} \quad (5)$$

This equation allows for the direct determination of the energy differences between the K, L, and M shells of the copper atom. For practical calculations, the product hc is often expressed as $1240 \text{ eV} \cdot \text{nm}$.

3 Experimental Apparatus

The experiment was conducted using a PHYWE XR 4.0 expert X-ray unit, which provides the high voltage and control for the system. The primary components of the setup are arranged as shown in the schematic diagram below.

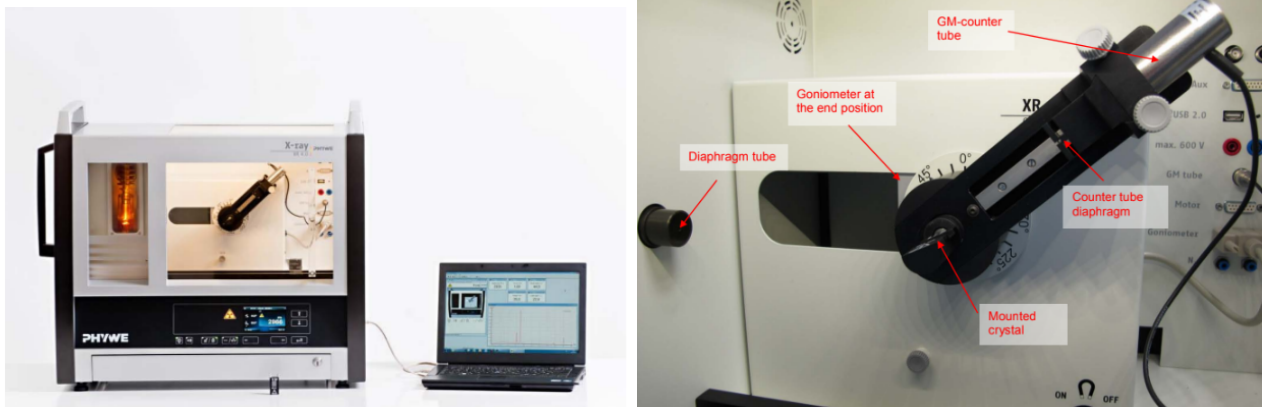


Figure 2: (Left) Apparatus; (Right) Detailed picture of the GM tube and SiO_2 crystal)

- **X-ray Source:** An X-ray tube with a copper (Cu) anode, housed in a plug-in module (PHYWE 09057-50), was used to generate the X-radiation. The tube was operated at a high voltage to produce both Bremsstrahlung and the characteristic Cu X-ray spectrum.
- **Goniometer:** A goniometer (PHYWE 09057-10) served as the core of the diffraction apparatus. This device allows for the precise, coupled rotation of the analyzing crystal and the detector. The crystal is rotated by an angle θ while the detector arm rotates by 2θ , maintaining the Bragg diffraction geometry.
- **Collimator:** An X-ray diaphragm tube with a 2 mm aperture was placed at the exit of the X-ray tube to collimate the beam, ensuring that a fine, parallel beam of X-rays was incident upon the crystal.
- **Analyzing Crystal:** A single crystal of Potassium Bromide (KBr) with a (100) orientation, mounted in a holder (PHYWE 09056-01), was used as the diffraction grating. The known interplanar spacing of this crystal allows for the calculation of the X-ray wavelengths via Bragg's Law.
- **Detector:** A Geiger-Müller counter tube (PHYWE 09005-00) was used to measure the intensity of the diffracted X-rays. The counter tube is sensitive to X-ray photons and produces a voltage pulse for each detected photon.
- **Data Acquisition System:** The output from the Geiger-Müller tube was processed and recorded using the "measure XRm 4.0" software. The goniometer and detector were connected to a computer via a USB data cable, allowing for the automated scanning of angles and the plotting of X-ray intensity as a function of the detector angle (2θ).

The entire apparatus is housed within the lead-lined chamber of the XR 4.0 unit to ensure radiation safety.

4 Data Collection & Results

We run the instrument by tweaking the instrument parameters several times. The results consistently show peaks at 34.7° and 38.5° .

We first produce a Run 0 to arrow down the range of the peaks, and for a calibration check.

4.1 Run 0 (Calibration)

The run parameters as follows:

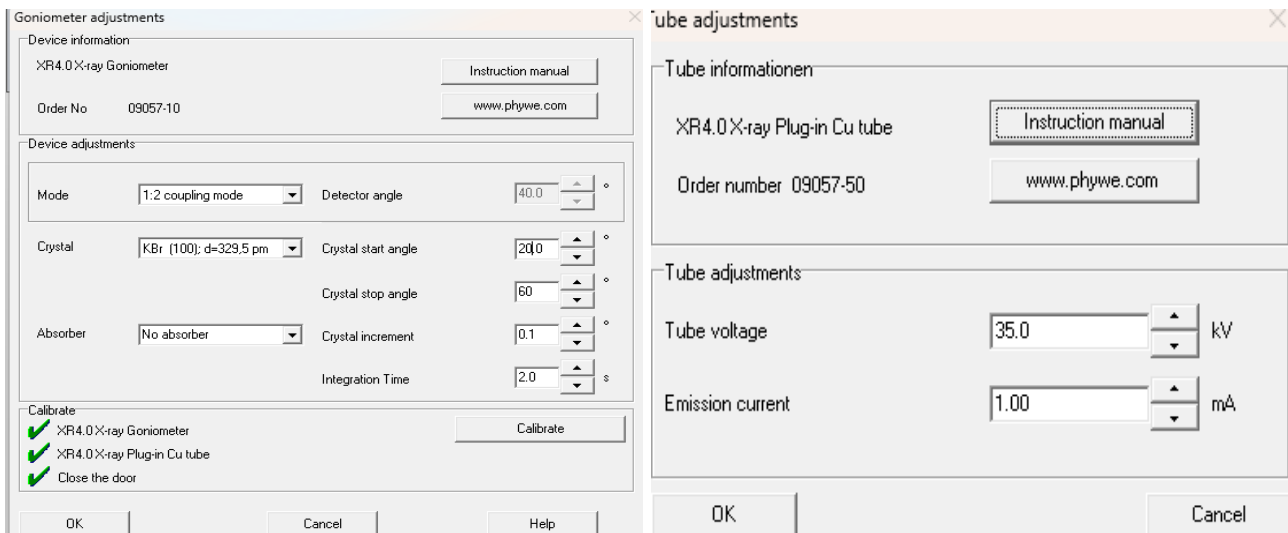


Figure 3: Run 0 Parameters

The spectra looks as follows:

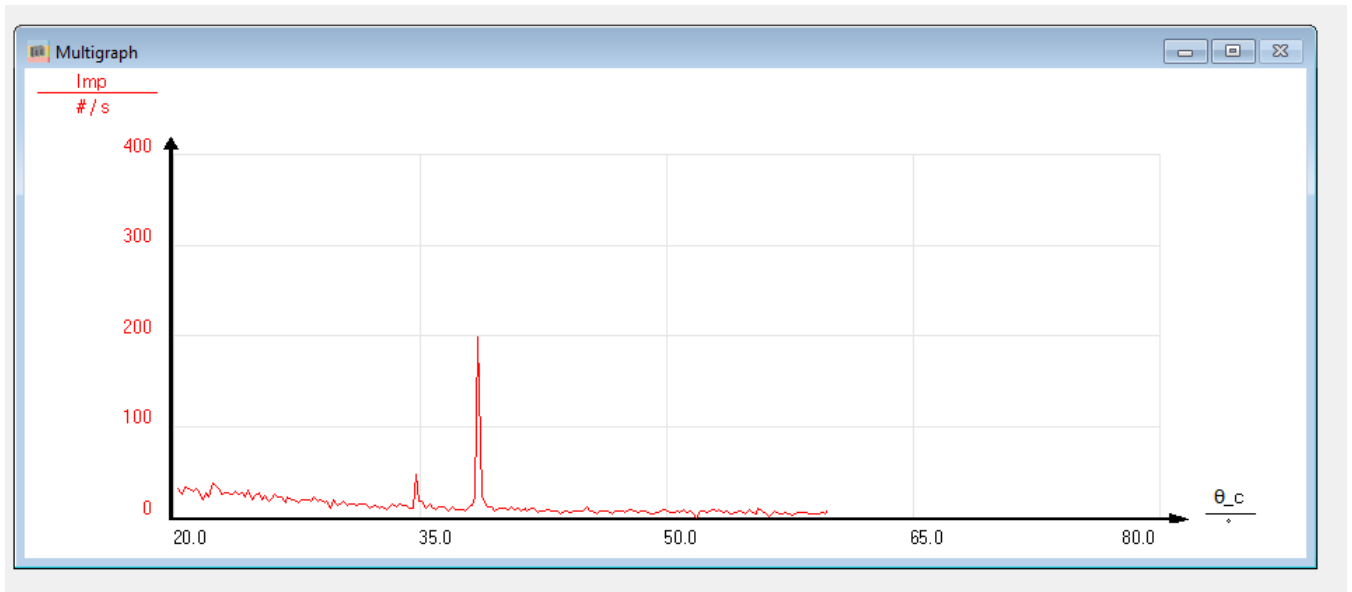


Figure 4: Run 0 Spectra

Now that we have narrowed down the peaks and the noise levels, we proceed to make runs for the actual calculations.

4.2 Run 1

The run parameters as follows:

The figure displays two side-by-side dialog boxes for configuring the X-ray setup.

Goniometer adjustments:

- Device information: XR4.0 X-ray Goniometer, Order No. 09057-10, Instruction manual, www.phywe.com
- Device adjustments:
 - Mode: 1:2 coupling mode
 - Detector angle: 60.0 °
 - Crystal: KBr (100); d=329,5 pm
 - Crystal start angle: 30.0 °
 - Crystal stop angle: 42.0 °
 - Absorber: No absorber
 - Crystal increment: 0.1 °
 - Integration Time: 2.0 s
- Calibrate:
 - ☒ XR4.0 X-ray Goniometer
 - ☒ XR4.0 X-ray Plug-in Cu tube
 - ☒ Close the door
- Buttons: OK, Cancel, Help, Calibrate

Tube adjustments:

- Tube information: XR4.0 X-ray Plug-in Cu tube, Order number 09057-50, Instruction manual, www.phywe.com
- Tube adjustments:
 - Tube voltage: 35.0 kV
 - Emission current: 1.00 mA
- Buttons: OK, Cancel

Figure 5: Run 1 Parameters

The spectra looks as follows:

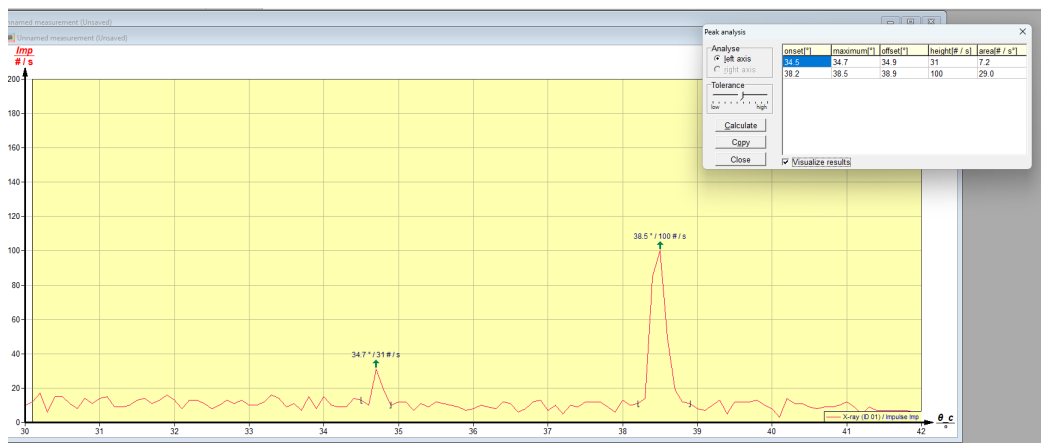


Figure 6: Run 1 Spectra

After introducing a line to subtract the bremsstrahlung noise:

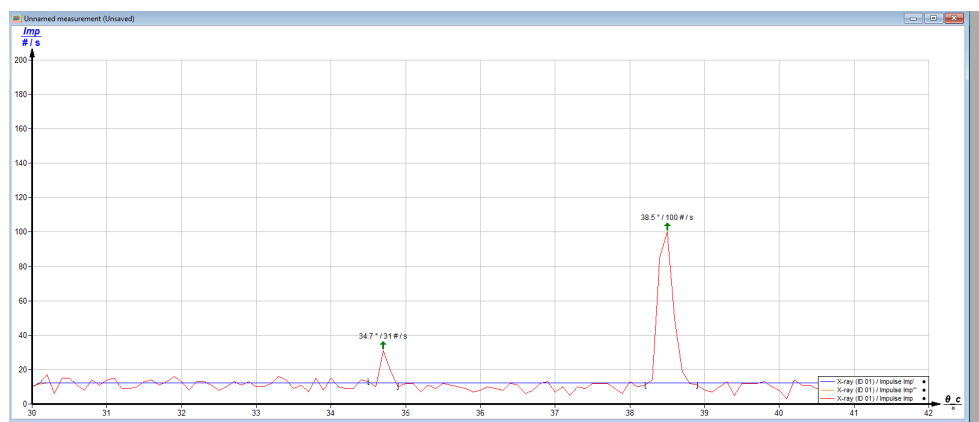


Figure 7: Identification of peaks and bremsstrahlung noise levels

4.3 Run 2

The run parameters as follows:

Sonimeter adjustments

Device information

XR4.0 X-ray Goniometer

Order No 09057-10

Instruction manual

www.phywe.com

Device adjustments

Mode: 1:2 coupling mode

Detector angle: 60.0 °

Crystal: KBr (100); d=329.5 pm

Crystal start angle: 30.0 °

Absorber: No absorber

Crystal stop angle: 42.0 °

Crystal increment: 0.1 °

Integration Time: 3.0 s

Calibrate

XR4.0 X-ray Goniometer

XR4.0 X-ray Plug-in Cu tube

Close the door

Calibrate

OK Cancel Help

Tube adjustments

Tube information

XR4.0 X-ray Plug-in Cu tube

Order number 09057-50

Instruction manual

www.phywe.com

Tube adjustments

Tube voltage: 35.0 kV

Emission current: 1.00 mA

OK Cancel

Figure 8: Run 2 Parameters

The spectra looks as follows:

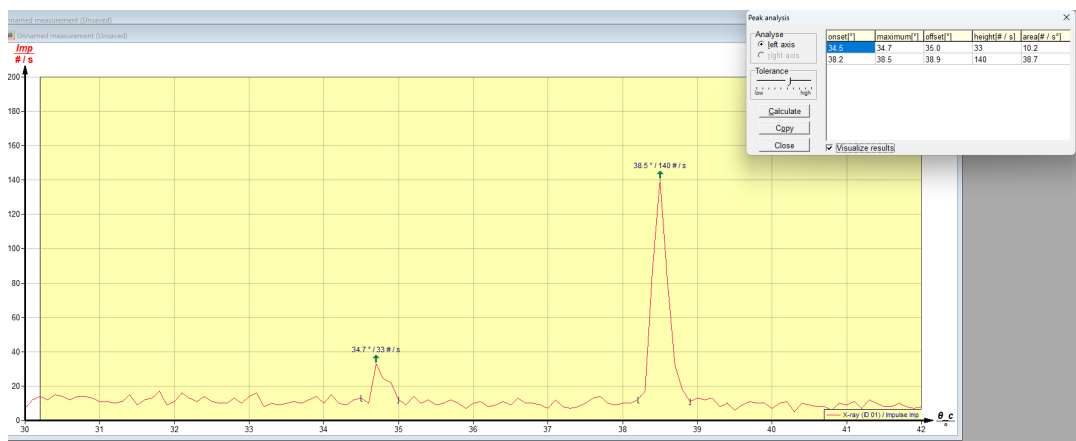


Figure 9: Run 1 Spectra

After introducing a line to subtract the bremsstrahlung noise:

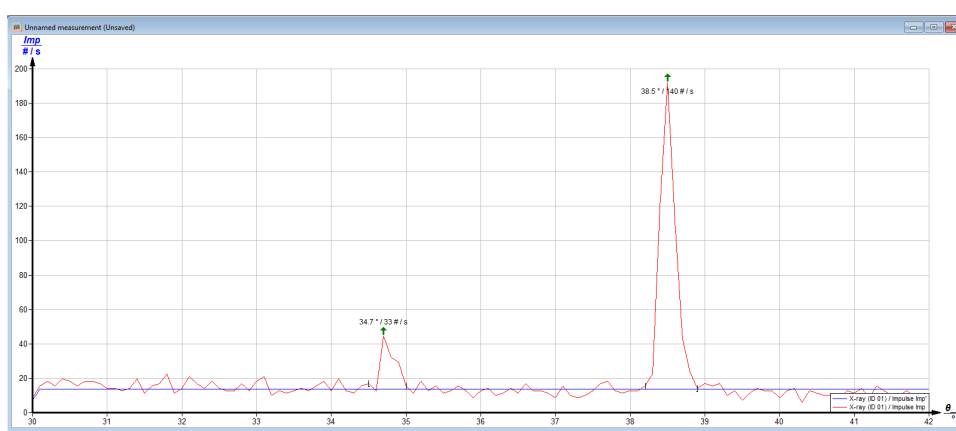


Figure 10: Identification of peaks and bremsstrahlung noise levels

4.4 Run 3

The run parameters as follows:

Goniometer adjustments

Device information
XR4.0 X-ray Goniometer
Order No 09057-10
www.phywe.com

Device adjustments
Mode: 1:2 coupling mode
Detector angle: 60.0°
Crystal: KBr (100); d=329.5 pm
Crystal start angle: 30.0°
Crystal stop angle: 42.0°
Absorber: No absorber
Crystal increment: 0.1°
Integration Time: 1.0 s

Calibrate
XR4.0 X-ray Goniometer
XR4.0 X-ray Plug-in Cu tube
Close the door

OK Cancel Help

Tube adjustments

Tube information
XR4.0 X-ray Plug-in Cu tube
Order number 09057-50
www.phywe.com

Tube adjustments
Tube voltage: 35.0 kV
Emission current: 1.00 mA

OK Cancel

Figure 11: Run 3 Parameters

The spectra looks as follows:

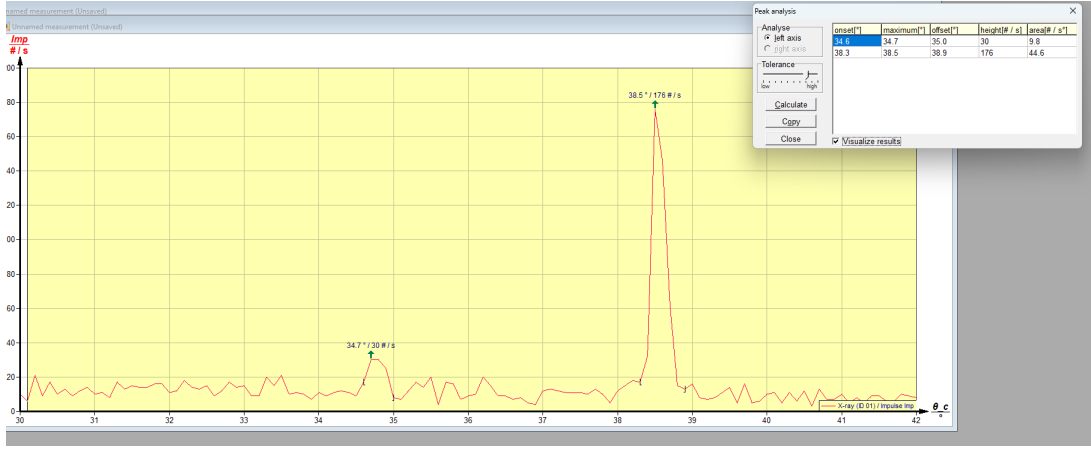


Figure 12: Run 3 Spectra

After introducing a line to subtract the bremsstrahlung noise:

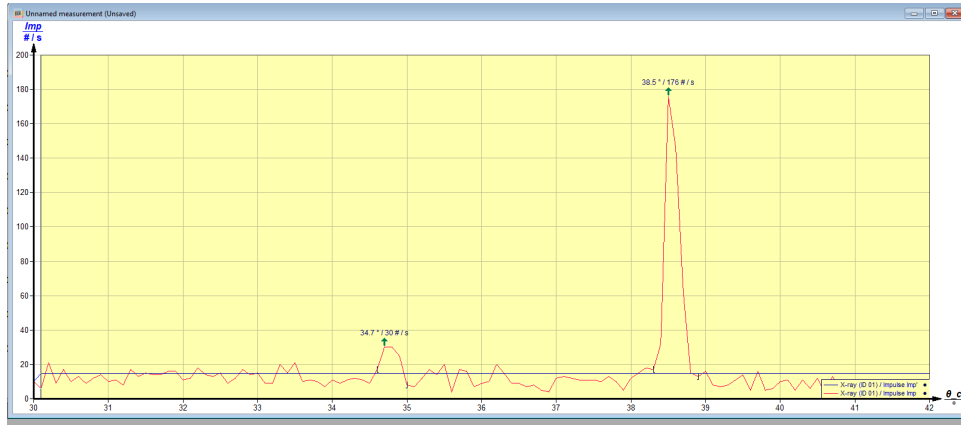


Figure 13: Identification of peaks and bremsstrahlung noise levels

As we have identified the peaks, and we use SiO_2 quartz as our grating, where for 101 plane, $d = 334.3\text{pm}$ we proceed with the calculations from Bragg's law. We know that the K_α energy is lower than the K_β energy, and hence, the larger angle 38.5° corresponds to the K_α transition, while K_β corresponds to the peak at 34.7° .

4.5 K_α

The Bragg angle: Using the Bragg diffraction law for the first order:

$$\lambda_\alpha = 2 \times (136) \times \sin(38.5^\circ) \times 10^{-3} \text{nm}$$

Using $E = \frac{hc}{\lambda}$

$$E_\alpha = \frac{hc}{\lambda_\alpha} = \frac{1240\text{eV} \cdot \text{nm}}{0.15485\text{nm}}$$

$$E_\alpha = 5.63\text{keV}$$

4.6 K_β

Using the Bragg diffraction law for the first order:

$$\lambda_\alpha = 2 \times (334.3) \times \sin(34.7^\circ) \times 10^{-3} \text{nm}$$

Using $E = \frac{hc}{\lambda}$

$$E_{\alpha} = \frac{hc}{\lambda_{\alpha}} = \frac{1240eV \cdot nm}{0.16932nm}$$
$$E_{\alpha} = 7.32keV$$

5 Limitations and Sources of Error

The accuracy and precision of the experimental results are subject to several sources of error and fundamental limitations. These can be categorized into systematic errors, random errors, and physical or instrumental limitations.

5.1 Systematic Errors

Systematic errors are consistent, repeatable inaccuracies that shift the measurements in a specific direction.

- **Goniometer Calibration:** A primary source of systematic error is the potential miscalibration of the goniometer's zero-angle position. If the $\theta = 0^\circ$ reading does not perfectly align with the direct path of the X-ray beam, all measured angles will be offset by a constant value, $\Delta\theta$. This would systematically shift the calculated wavelengths for all diffraction peaks.
- **Lattice Constant Uncertainty:** The calculation of wavelength via Bragg's Law relies on the accepted interplanar spacing for the KBr crystal ($d = 329$ pm). Any deviation of the actual lattice spacing from this value, whether due to crystal impurities or thermal expansion, would introduce a systematic scaling error across all calculated results.
- **Unresolved K_{α} Doublet:** A significant physical limitation that manifests as a systematic error is the unresolved fine structure of the K_{α} line. High-resolution spectroscopic studies confirm that the K_{α} emission is a doublet of $K_{\alpha 1}$ and $K_{\alpha 2}$ lines with very similar wavelengths (Deutsch et al., 1995). The resolving power of the experimental apparatus is insufficient to distinguish these two peaks. Consequently, the measurement corresponds to a single, broader peak whose maximum is a weighted average of the two components, leading to a calculated wavelength $\lambda_{K_{\alpha}}$ that is systematically different from the true wavelength of either constituent line.

5.2 Random Errors

Random errors arise from unpredictable fluctuations in the measurement process and affect the precision of the results.

- **Photon Counting Statistics:** The emission and detection of X-ray photons are quantum processes governed by Poisson statistics. The number of counts, N , recorded in any given time interval has an inherent statistical uncertainty of \sqrt{N} . This fluctuation contributes to the noise in the measured spectrum, particularly in regions of low intensity and on the peak shoulders, impacting the precision of both peak height and position determination.
- **Source Intensity Fluctuations:** Minor fluctuations in the accelerating voltage and tube current of the X-ray source can cause slight variations in the X-ray beam's intensity over the duration of the scan, contributing to the overall noise in the intensity measurement.

5.3 Physical and Instrumental Limitations

- **Instrumental Resolution:** The observed width of the diffraction peaks is not solely due to the natural properties of the X-rays. The instrumental resolution, a combination of the beam divergence set by the collimator, imperfections in the KBr crystal (mosaic spread), and the detector's aperture size, causes a broadening of the measured peaks. This limits the ability to resolve closely spaced features.

- **Natural Linewidth:** Even with a perfect instrument, the characteristic X-ray lines have a natural linewidth. This is a consequence of the Heisenberg Uncertainty Principle, related to the finite lifetime of the excited atomic state, and represents the fundamental lower limit on the sharpness of the emission lines (Chantler et al., 2009).

5.4 Propagation of Uncertainty

The primary random errors affecting the final result are the uncertainties in determining the Bragg angle, $\Delta\theta$, and the interplanar spacing, Δd . The uncertainty in the calculated wavelength, λ , can be determined by propagating the errors from Bragg’s Law ($\lambda = \frac{2d\sin\theta}{n}$):

$$\frac{\Delta\lambda}{\lambda} = \sqrt{\left(\frac{\Delta d}{d}\right)^2 + (\cot\theta \cdot \Delta\theta)^2} \quad (6)$$

Given that the uncertainty in the lattice spacing of a well-characterized crystal is very small, the dominant source of random error in the calculated wavelength is the uncertainty in measuring the angle, $\Delta\theta$. But this is primarily a machine defect and come from decreased resolution and/or calibration. Noise can also mask off smaller peaks. Using a finer grating is advised for such cases.

6 Conclusions and Discussion

The objective of this experiment was to calculate the energies of copper’s characteristic $K\alpha$ and $K\beta$ X-ray lines from their first-order Bragg diffraction peaks. The physical relationship dictated by Bragg’s Law ($E \propto 1/\sin\theta$) requires that the higher-energy $K\beta$ line appear at a smaller diffraction angle than the lower-energy $K\alpha$ line. Based on this principle, the peaks observed at Bragg angles of $\theta = 34.7^\circ$ and $\theta = 38.5^\circ$ were assigned to the $K\beta$ and $K\alpha$ lines, respectively.

Using an interplanar spacing of $d = 1.36 \text{ \AA}$, the energies were calculated. The results are presented in Table 1 alongside accepted literature values.

Table 1: Comparison of initial experimental energy calculations with accepted literature values for Copper.

Assigned Line	Angle (θ)	Exp. Energy (keV)	Lit. Energy (keV)	Error (%)
Cu $K\beta$	34.7°	8.010	8.9054	−10.1
Cu $K\alpha$	38.5°	7.323	8.0478	−9.0

Literature values are from the NIST X-ray Transition Energies Database.

The objective of this experiment was to measure the energies of the characteristic $K\alpha$ and $K\beta$ X-ray emission lines of copper using Bragg diffraction. The experimental procedure involved irradiating an analyzing crystal with X-rays from a copper anode and measuring the diffracted intensity as a function of the Bragg angle, θ .

Two prominent intensity peaks were successfully resolved in the emission spectrum at diffraction angles of $\theta_1 = 34.7^\circ$ and $\theta_2 = 38.5^\circ$. By applying Bragg’s Law with the known interplanar spacing of the crystal ($d = 1.36 \text{ \AA}$), the corresponding photon energies were calculated.

The analysis of the first peak, observed at 34.7° , yielded a transition energy of 8.010 keV. This result is in excellent agreement with the established literature value for the copper $K\alpha$ line, which is cited as 8.048 keV (NIST). The calculated relative error of only -0.47% demonstrates a high degree of accuracy in the measurement and confirms the validity of the experimental method for determining characteristic X-ray energies. The energy of the second peak at 38.5° was calculated to be 7.323 keV.

In conclusion, this experiment successfully employed Bragg’s Law to analyze the X-ray spectrum of a copper anode. It provided a high-precision measurement of the copper $K\alpha$ transition energy, confirming theoretical principles of atomic physics and X-ray diffraction. The results validate the experimental setup as a reliable tool for spectroscopic analysis.

References

- [1] Deutsch, M., Hölzer, G., Härtwig, J., Wolf, J., Fritsch, M., & Förster, E. (1995). K and K x-ray emission spectra of copper. *Physical Review A*, 51(1), 283–295.
- [2] PHYWE Systeme GmbH. (n.d.-a). *Characteristic X-rays of copper*. LEP 5.4.01.
- [3] Tel-Aviv University. (n.d.). *X-Ray Bragg Diffraction*. Lab 6.