By means of Bragg's Law; determining the wavelengths of the characteristic Kα and Kβ radiation of molybdenum.

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Abstract:

This experiment was performed to determine the wavelengths for the characteristic Kα and Kβ transition lines of the Molybdenum atoms by x-ray radiation and hence authenticate the validity of Bragg's Law, confirming the wave nature of x-rays. Our results for the mean value of the characteristic wavelength λ for Kα and Kβ were 70.76 ± 1.35 pm and 62.94 ± 1.36 pm respectively. These results with their corresponding standard deviation were very close to the literature Kα and Kβ values, 71.08pm and 63.09pm.

Keywords: X-rays, NaCl monocrystal, Diffraction, Wavelength, Bragg's Law

PACS:

Introduction:

Photons, which are packets of energy, always move with the universal speed of light. One way to describe electromagnetic radiation is in terms of photons, where the flow of photons through space is known as electromagnetic radiation. Near the end of the 19th century, a German physicist by the name of Wilhelm Conrad Rontgen, formed and detected, electromagnetic radiation in a wavelength understood as x-rays while experimenting with cathode ray tubes-vacuum tubes. Scattering from a solid can polarize x-rays because of their wave nature. With the aid of X-rays, Sir W. L. Bragg and his son W. L. Bragg set about experimenting what would happen if a series of irregular impulses fell on diffracting points arranged on a regular space lattice. [1]. Moreover, because of x-rays shorter wavelengths, it gave them a vision into the actual arrangement of the atoms in solid bodies, which led them to observe the crystal pattern arranged on a space lattice. An ionic crystal consists of ions bound together by electrostatic attraction. When these ions are arranged in a regular, geometric structure we call it a crystal lattice. One example of a compound displaying these characteristics is NaCl monocrystal.

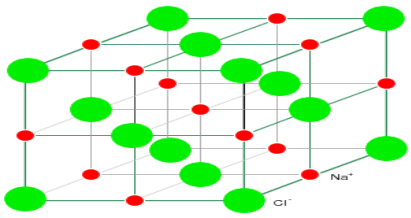

Figure 1: NaCl structure; Red - Sodium ions and Green - Chloride ions. [4].

As stated by the Bragg's, the points of such kind of a space lattice could be arranged in series of planes, parallel and equal distances from each other. By passing a pulse over each diffracting point, the scattering of a wave occurs. Also known as the Hugyens' Principle, if a number of points are arranged on a plane the diffracted wavelets will then combine to form a reflected wave front.

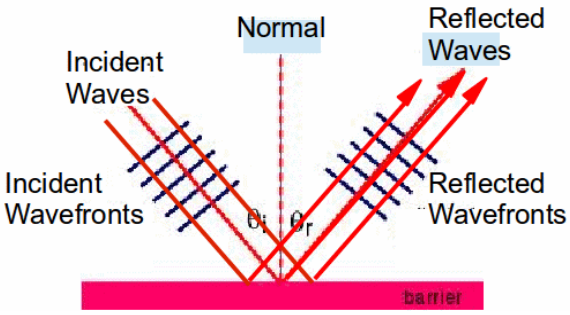

Figure 2: Reflection of Waves. [6].

Experimental Design:

The measurements in our experiment are managed using the built in goniometer of the x-ray apparatus. These x-rays are detected using a Geiger – Muller counter that a voltage is applied and filled with an inert gas such argon at low pressure. Constructive interference occurs in the x-rays reflected at the individual lattice planes when their path differences, Δ are integral multiples of the wavelength

$$\Delta = n * \lambda \qquad (1)$$

where n = 1, 2, 3, … .

For two adjacent lattice planes with spacing d, the incident and reflect rays with θ for the path differences Δ_1 and Δ_2, becomes

$$\Delta_1 = \Delta_2 = d * \sin\vartheta$$

Hence, the total path difference is

$$\Delta = 2 * d * \sin\vartheta$$

Equation (1) and (3) combine to give us The Bragg's Law of reflection

$$n * \lambda = 2 * d * \sin\vartheta \quad (2)$$

where n is an integer, λ is the wavelength of the incident X-ray beam, d is the spacing between two adjacent planes. And the angle ϑ is known as the glancing angle or the angle of incidence.

The standard deviation of the wavelengths λ were estimated by

$$\sigma_\lambda = \lambda \frac{\sigma_\vartheta}{\vartheta}. \quad (3)$$

The x- ray radiation consists of sharp spikes, also known the characteristic lines, which are caused by electrons being knocked out of the K shell of an atom and then the electrons from the L shell fall down into the vacancies in the K shell. [3]. This results in the energy being emitted in the form of K alpha and K beta lines. To

investigate Bragg's law, we used the Kα and Kβ transitions of the molybdenum atoms. The element Molybdenum, is a metallic element found in nitrogen-fixing bacteria.[2]. Some of its properties are given below in the table,

Table 1: Energy E, frequency v, and wavelength λ of the characteristic x-ray radiation of molybdenum

keV = 10^3 eV, EHz = 10^{18} Hz, pm = 12^{-10}m

	E / keV	v / Ehz	λ / pm
Kα	17.443	4.2264	71.08
Kβ	19.651	4.8287	63.095

For our NaCl moncrystal, the lattice spacing, d, = 282.01 pm. The corresponding glancing angles at which the diffraction maxima are expected for scattering for this crystal up to the third order diffraction are stated below,

Table 2: Glancing angle ϑ of the characteristic x-ray radiation of molybdenum for diffraction at an NaCl monocrystal up to the third order

n	ϑ (Kα)	ϑ (Kβ)
1	7.24^o	6.42^o
2	14.6^o	12.93^o
3	22.21^o	19.61^o

The values given in Table 1 and Table 2 are our literature values, [5], or theoretical values so as to speak. In our conclusion, we will make the comparison between these literature and our experimental values to validate our results. The data is transmitted to the PC via the RS-232 serial interface on the x-ray apparatus. We then used the software "X-ray Apparatus" to record, display and evaluate the data supplied by the x-ray apparatus.

Experimental Results:

We started off by setting the x-ray high voltage U = 35.0kV, the emission current I = 1.00mA, and the measuring time per angular step Δt = 10s, with the angular step width $\Delta\beta = 0.1^{o}$. Then we proceeded by pressing the COUPLED key on the device to enable 2ϑ coupling of the target and the sensor, and setting the lower limit value of the target angle to 2^{o} and the upper limit to 25^{o}. We selected these limits to make sure that three sets of peaks we obtained were captured in our data. By pressing the SCAN key, we started the measurement and data transmission to the PC. When the measurements were finished we obtained the following diffraction spectrum of x-ray radiation for Bragg reflection to the third order at a NaCl monocrystal.

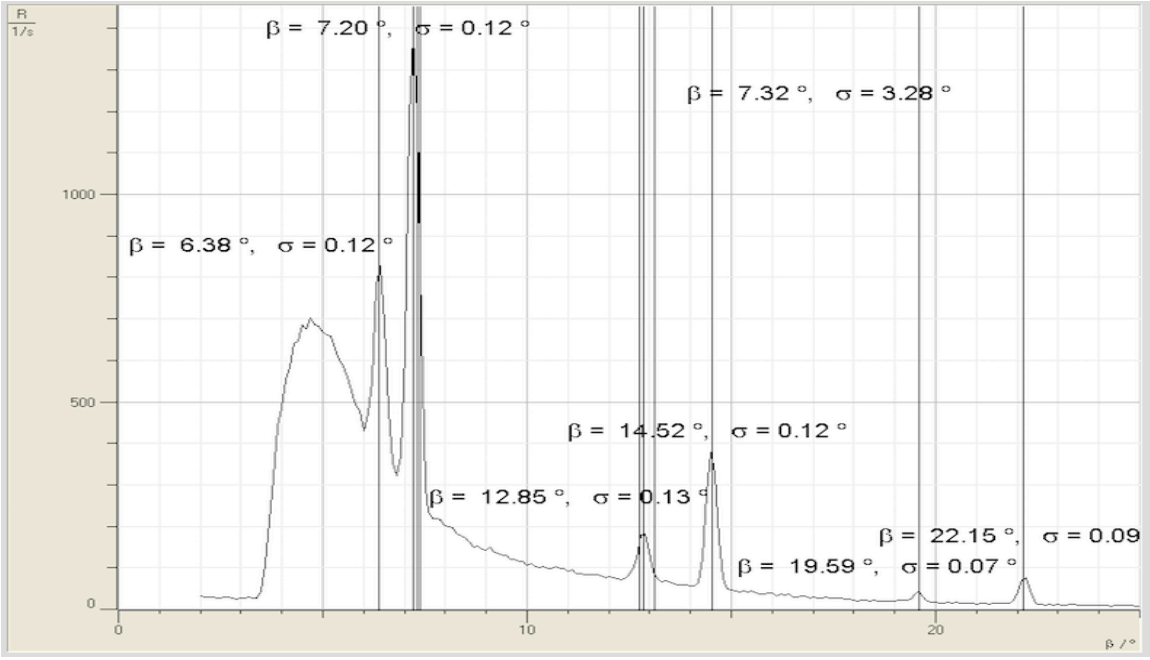

Figure 3: Containing three sets of peak, where each of the first peaks is the Kα peak and the second peak is Kβ peak. Above each peak is the corresponding angle marked as β, which is an arbitrary symbol assigned by the x-ray program used in the experiment and for the purposes of this experiment will be regarded as ϑ in accordance with Bragg's law, with standard deviation σ.

By using the glancing angles ϑ of the Molybdenum Kα and Kβ lines, and the lattice plane spacing d = 282.01 pm, we calculated the wavelength λ using Bragg's law of reflection given by equation (2), and the uncertainty in wavelength λ by using equation (3). By the help of the X-ray software, we obtained the uncertainties for our glancing angles ϑ for the Kα and Kβ lines.

Table 3: Measured glancing angles of the Mo Kα line and the calculated wavelengths λ for the first through third diffraction orders

n	ϑ (Kα)	λ (Kα)/pm	σ in wavelength
1	7.20±0.12°	70.69	1.18
2	14.52±0.12°	70.70	0.58
3	22.15±0.09°	70.88	0.29

Table 4: Measured glancing angles of the Mo Kβ lines and the calculated wavelengths λ for the first through third diffraction orders

n	ϑ (Kβ)	λ (Kβ)/pm	σ in wavelength
1	6.38±0.12°	63.07	1.19
2	12.85±0.13°	62.72	0.63
3	19.59±0.07°	63.04	0.23

For our individual diffraction orders of the measured wavelengths, we calculated the mean values. The following values were obtained

$$K\alpha = 70.76 \pm 1.35 \text{ pm}$$

and

$$K\beta = 62.94 \pm 1.36 \text{ pm},$$

Where the standard deviation of Kα and Kβ was calculated in quadrature with the three previous standard deviations of each (given in Tables 3 and 4, respectively).

Conclusion:

We obtained the Kα and Kβ wavelength values to be 70.76 ± 1.35 pm and 62.94 ± 1.36 pm respectively. Our experimentally determined wavelengths λ for the characteristic lines are very close to the literature values for Kα and Kβ that are 71.08pm and 63.10pm, respectively. We conclude our results as precise, hence certifying Bragg's Law of diffraction.

Acknowledgments:

I would like to thank Professor Carolyn MacDonald, whose course of X-ray Optics, which I'm currently taking. It has helped me develop a better understanding of x-ray radiation and the transitional energies associated with elements such as Molybdenum, which we used in this experiment.

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