Using Bragg Diffraction to find the Wavelength of X-Rays and the Density of MgO

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The goals of the experiments were to use Bragg diffraction of x-rays on crystals of LiF, MgO (100), and MgO (110) in order to obtain the characteristic wavelength of the x-rays produced from copper and to determine the density of MgO. The measurements were made by sending x-rays toward the crystals at various angles while a counter counted the number of x-rays that were reflected toward it by the crystals. Certain angles for each crystal produced a large amount of counts. By finding the angle where many counts occured, the characteristic wavelength of the x-rays, and the density of MgO could be calculated. I obtained a value of $1.567 \pm 0.002\mathring{A}$ for the characteristic wavelength of x-rays produced by copper which corresponds to a 2% error from the accepted value of $1.54\mathring{A}$. The density of MgO was calculated from using both MgO (100) and MgO (110) and I obtained values of 3.58 ± 0.02 g/cm^3 and 3.64 ± 0.03 g/cm^3. The accepted value for the density of MgO is 3.58 g/cm^3 which agrees with my first result and my second result has a 2% error from this value. These results verify Bragg's theory of x-ray diffraction with crystalline objects that won him the Nobel Prize in 1915. This theory is now known as Bragg's law.

I. INTRODUCTION

Crystalline objects like diamonds are sought after because of their unique structures and overall beauty. However, it wasn't until the beginning of the twentieth century that the true nature of the structures within crystals was discovered. The method of x-ray diffraction for studying crystal structures was developed by Max von Laue and won him the 1914 Nobel Prize in Physics[1]. William Lawrence Bragg expanded on this work in that he theorized what is now known as Bragg's law. He and his father, William Henry Bragg, won the 1915 Nobel Prize in Physics for this work and led to an increased understanding of cyrstalline structures[2].

Several experiments were performed in order to determine the x-ray spectrum of copper and the crystalline structure of magnesium oxide (MgO). The goals of the first two experiments were to use Bragg diffraction off of lithium fluoride (LiF) in order to determine the x-ray spectrum of copper, which has an accepted value of 1.54 $\mathring{A}^3$. The goal of the last two experiments were to find the density of MgO by finding the lattice spacing of MgO (100) and MgO (110). The density of MgO has an accepted value of 3.58 g/cm^3[4]. Being able to determine these values will help verify Bragg's law and allow for a greater understanding of the structure of these crystals.

II. THEORY

A. Characteristic and Bremsstrahlung X-Rays

Characteristc and bremsstrahlung x-rays are produced when a metal like copper is bombarded with high speed electrons. When the bombarding electrons eject the electrons from the inner shells of the atoms, the vacancies are filled by electrons from higher levels dropping down. This action results in the emitting of characteristic x-rays which have sharply defined frequencies. Bremsstrahlung x-rays are different in that they are emitted when electrons are decelerated; due to being fired at a metal. These x-rays have a broad range in wavelength because they are dependent on the degree to which the electrons were decelerated. Thus, characteristic wavelengths are prefered due to their well defined frequencies[5].

B. Finding Lattice Spacing of LiF with Known Quanitities

The mass of a molecule of LiF can be written as

$$Mass = \frac{M}{N}, \tag{1}$$

where M is the molecular weight of LiF and N is Avogadro's number which have values of 25.939 g/mol and 6.02×10^{23} molecules/mol, respectively[6].

The number of LiF atoms per unit of volume, v, is given as

$$v = \frac{2\rho N}{M}, \tag{2}$$

where the density, ρ, of LiF is known to be 2.64 g/cm^3[6].

Since the volume is the lattice spacing cubed, Eqn. 2 can be rewritten as

$$d = \sqrt[3]{\frac{M}{2\rho N}}. \tag{3}$$

C. Finding λ of Characteristic and Bremsstrahlung X-Rays

An incident plane of characteristic and bremsstrahlung x-rays will be scattered by the atoms within the crystal

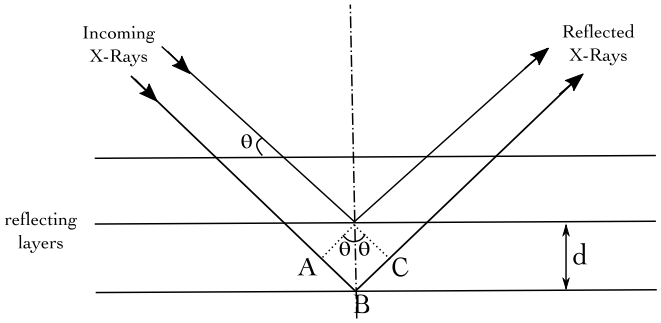

FIG. 1. The physical phenomena of x-rays reflecting off of different layers of a crystal. The beam hitting the second layer will be a distance $2d\sin\theta$ ahead of the lower beam. The extra distance traveled by the lower beam is noted by the segments $\overline{AB}$ and $\overline{BC}$ which are equal in length due to geometry. If the beams coming in are at a particular θ such that the beam difference is equal to an integer mulitple of the wave's wavelength, the beams will interefere constructively and yiel a maxima of intensity.

and a portion of the beam is reflected by the various planes of the crystal (see Fig. 1). Fig. 1 reveals that the beam reflected by the third layer travels a distance $2d\sin\theta$ more than the beam reflected by the second layer. If the path difference between these beams is equal to the wavelength of the rays multiplied by a positive integer, n, the beams will interefere constructively and result in a maxima of intensity[7]. This can be written as:

$$n\lambda = 2d\sin\theta, \tag{4}$$

where n is the wave number, θ is the angle with respect to the surface of the crystal, and d is the lattice spacing distance.

Thus, by finding the values of θ at which the beams constructively interfere and yield maxima of intensity, and by using Eqn. 3 to find the lattice spacing distance, d, of the crystal, the wavelengths of the characteristic and bremsstrahlung x-rays can be calculated using the following formula derived from Eqn. 4:

$$\lambda = \frac{2d\sin\theta}{n}. \tag{5}$$

D. Finding the Density of MgO

Knowing the wavelength of the x-rays allows for the lattice spacing, d, to be calculated by rewriting Eqn. 4 as

$$d = \frac{n\lambda}{2\sin\theta}. \tag{6}$$

By knowing d, it is possible to calculate the density, ρ, of MgO. By rewriting Eqn. 3 the following formula is obtained:

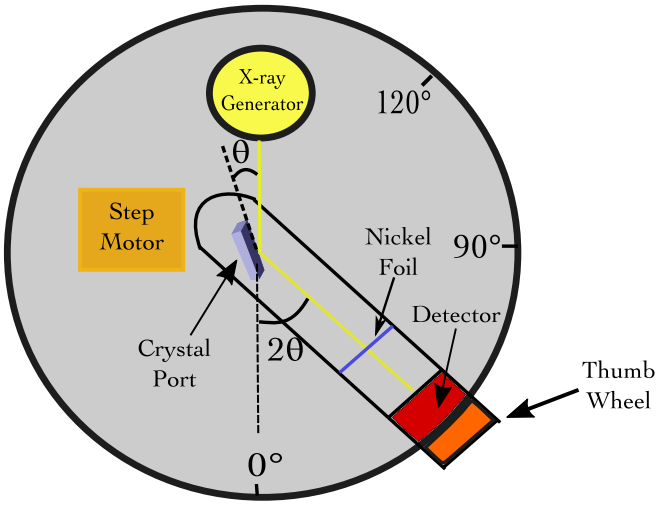

FIG. 2. A top view of the apparatus used for x-ray diffraction off of crystals. The x-rays are produced by sending high speed electrons at a copper target. A crystal is put into the crystal port and the xrays head toward it. These x-rays are reflected toward the detector on the arm. The arm is controlled by a step motor which is connected to a computer (not shown) to control its movement. A nickel plate can be added in front of the detector in order to absorb the bremsstrahlung wavelengths.

$$\rho = \frac{M}{2Nd^3}. \tag{7}$$

III. EXPERIMENT

The apparatus used for the experiments is shown in Fig. 2. The apparatus is connected to a computer which controlled the step motor. The step motor was used to move the arm which, in turn, rotates the crystal in the crystal port. A detector at the end of the arm detected the number of x-rays hitting it and the number of counts was outputted to a program in MatLab. The procedure for each experiment was the following:

1. Put appropriate crystal into the crystal port
2. Move arm back to 0° and then move forward to 15° (Remove backlash)
3. Turn on x-ray generator
4. Run Matlab program

For the first experiment, the LiF crystal was used and no nickel plate was used in order to obtain peaks from both the bremsstrahlung and characteristic wavelengths. The second experiment was similar to the first but the only difference was that the nickel plate was used in order to absorb the bremsstrahlung wavelength and only leave the characteristic wavelength. The final two experiments

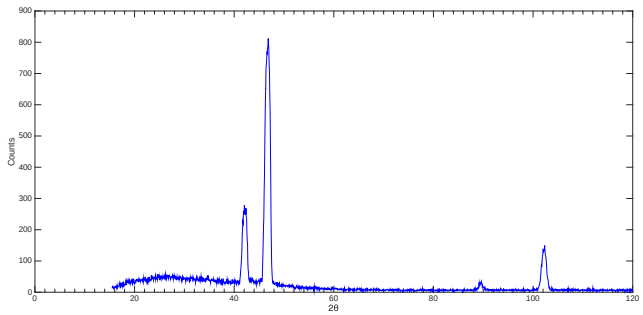

FIG. 3. This graph reveals the amount of x-rays counted by the detector over a wide range of angles. The crystal that was used was LiF and no nickel plate was used. The peaks at 42.1 ± 0.2 deg and 89.5 ± 0.2 deg correspond to bremsstrahlung wavelengths while the peaks at 46.4 ± 0.4 deg and 100.7 ± 0.2 deg correspond to characteristic wavelengths.

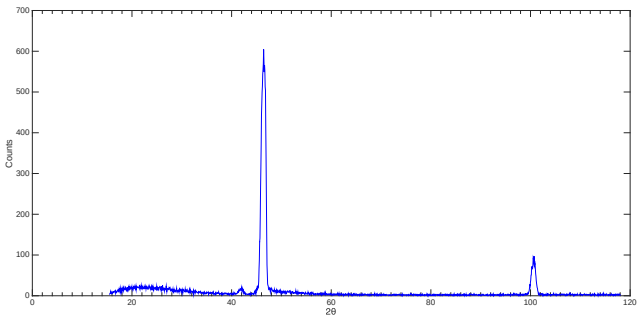

FIG. 4. This graph is the amount of x-rays counted by the detector over many values of 2θ. The crystal that was used was LiF and the nickel plate was used as well. The peaks occur at angles of 46.4 ± 0.4 deg and 100.7 ± 0.2 deg. These peaks correspond to the characteristic wavelength of the x-rays.

used crystals MgO (100) and MgO (110) and the nickel plate was used for both.

IV. RESULTS

A. LiF - No Nickel Plate

The results from using x-ray diffraction on LiF without the nickel plate are shown in Fig. 3. The peaks that correspond to bremsstrahlung wavelengths are seen at values of 2θ of 42.1 ± 0.2 deg and 89.5 ± 0.2 deg. The first and second peak correspond to values of $n = 1$ and$n = 2$, respectively. Using Eqn. 5 for each peak, I obtained two values of λ and averaged them in order to obtain a value for λ of $1.432 \pm 0.001 \mathring{A}$. The error was calculated by using the following equation:

$$\delta\lambda = \frac{1}{2\sqrt{(\delta\lambda_1)^2 + (\delta\lambda_2)^2}}, \tag{8}$$

where $\delta\lambda_1$ and $\delta\lambda_2$ are the error in the calculations of λ for each peak before averaging them together. These errors were determined to be the error in $\sin\theta$ which is

$$\delta \sin\theta = \delta\theta \cos\theta. \tag{9}$$

B. LiF - With Nickel Plate

The results from using x-ray diffraction on LiF with the nickel plate are shown in Fig. 4. The peaks associated with the bremsstrahlung wavelengths are gone due to the nickel plate absorbing them. The first peak, $n = 1$, has a value of 2θ of 46.4 ± 0.4 deg. The second peak, $n = 2$, has a value of 2θ of 100.7 ± 0.2 deg. Using Eqn. 5 for each peak, I obtained two values of λ and averaged them in order to obtain a value for λ of $1.567 \pm 0.002 \mathring{A}$. The error was determined by using Eqn. 8. The accepted value for the characteristic x-ray wavelength from copper is $1.54 \mathring{A}$. Although my value doesn't overlap with the accepted value, it does correspond to a 2% error.

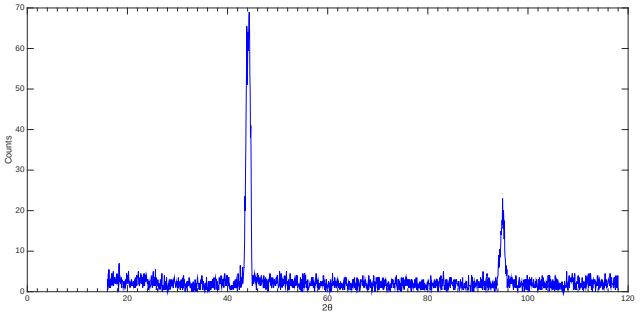

FIG. 5. The graph of the number of x-rays detected by the detector over a wide spread of angles. The crystal that was used was MgO (100) and the nickel plate was also used. The peaks occur at values of 2θ of 44.2 ± 0.2 deg and 94.9 ± 0.1 deg

C. MgO (100)

The results from using x-ray diffraction on a crystal of MgO (100) are shown in Fig. 5. The peaks for $n = 1$ and $n = 2$ occur at values of 2θ of 44.2 ± 0.2 deg and 94.9 ± 0.1 deg, respectively. Using Eqn. 6, I obtained a value of d of $2.105 \pm 0.008 \mathring{A}$. The error in d was determined to be

$$\delta d = \frac{nd\sqrt{(\delta\lambda/\lambda)^2 + (\delta \sin\theta / \sin\theta)^2}}{2} \tag{10}$$

By using a value of M of 40.3044 g/mol for MgO and Eqn. 7, ρ for MgO was calculated to be 3.58 ± 0.02 g/cm^3, where the error was determined to be

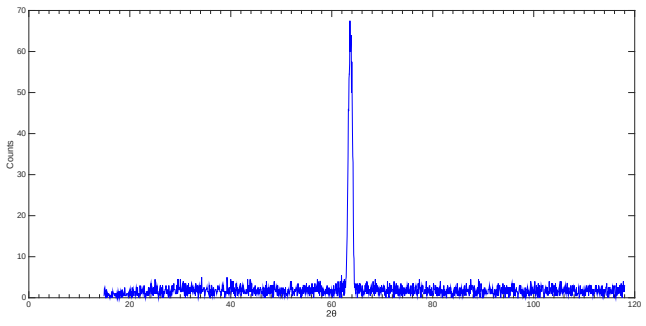

FIG. 6. The graph of the number of x-rays detected by the detector over a wide spread of angles. The crystal that was used was MgO (110) and the nickel plate was also used. The peak occurs at values of 2θ of 63.6 ± 0.2 deg.

$$\delta\rho = \frac{3\rho\delta d}{2d}. \tag{11}$$

The accepted value for ρ for MgO is 3.58 g/cm^3 which is exactly what I got with less than 1% uncertainty.

D. MgO (110)

The results from using x-ray diffraction on a crystal of MgO (110) are shown in Fig. 6. The peak for $n = 1$ occurs at a value of 2θ of 63.6 ± 0.2 deg. Using Eqn. 6 and multiplying this result by $\sqrt{2}$ yielded a value for d of $2.093 \pm 0.003\mathring{A}$. Multiplying by $\sqrt{2}$ was necessary because of the orientation of the planes in the MgO (110) crystal. Using Eqn. 7 and plugging in my calculated value of d for this crystal yielded a value for ρ of 3.64 ± 0.02 g/cm^3. This result does not overlap with the accepted value of 3.58 g/cm^3 but does correspond to an error of less than 2% from the accepted value.

V. CONCLUSIONS

I was successfully able to use Bragg diffraction of x-rays off of LiF in order to determine the characteristic wavelength of the x-rays produced by bombarding copper with electrons. The value for the wavelength I obtained has a value of $1.567 \pm 0.002\mathring{A}$ which corresponds with an error of 2% from the accepted value of $1.54\mathring{A}$. Using crystals of MgO (100) and MgO (110) I obtained values for the density of MgO of 3.58 ± 0.02 g/cm^3 and 3.64 ± 0.02 g/cm^3, respectively. My first value of ρ is exactly what the accepted value is for MgO and has an uncertainty of less than 1%. The second value of ρ doesn't overlap with the accepted value of 3.58 g/cm^3, but corresponds to a 2% error from the accepted value. These results verify that Bragg diffraction can be successfully implemented in order to determine lattice structures of crystals. Future work could involve using crystals that produce more than 2 peaks from characteristic wavelengths with the apparatus that was used. Crystals like NaCl are known to produce many peaks, which would allow for graphing n vs. $\sin\theta$ in order to obtain the lattice spacing.

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