Determining the distance between the planes of a model crystal lattice using Bragg’s Law

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Abstract

Bragg’s Law provides a means of explanation when investigating a crystal structure by relating the space between the spheres to the scattering angles of microwaves. This lab explored the phenomenon of Bragg diffraction by looking at the distances between the planes of a three dimensional crystal lattice. Using a microwave emitter, microwave were projected onto the crystal lattice, and then a receiver measured the reflectance intensity at various angles. The actual value of the distance between the planes of the crystal lattice was found to be 0.038 ± 0.001 m; and the average of the experimental values for the distance between planes was found to be 0.0381 ± 0.0014 m.
W.L. Bragg and W.H. Bragg were the first to derive the condition known as Bragg’s Law from diffraction experiments. Their services in the analysis of crystal structure won, both father and son, the Nobel Prize in Physics in 1915. W.L. Bragg was twenty-five years old when at the time of receiving the honor, which made him the youngest Nobel Prize winning Laureate.\textsuperscript{1} Bragg’s law utilizes the relationship between wavelength, and diffraction angles to find the spacing between two atomic planes.\textsuperscript{2} The atomic structure is not visible with a naked eye, so the concept of Bragg diffraction can be a dis-familiar; so in order to make the idea of Bragg diffraction less conceptual and more hands-on, macroscopic Bragg labs have been created, in the order of centimeters, to demonstrate the idea of Bragg diffraction.

Undergraduate labs covering Bragg diffraction are available on the web, this lab PASCOs Microwave Optics Lab, experiment 12: Bragg diffraction.\textsuperscript{3} The instruction and equipment preparation of the PASCO lab are clear and concise, making the PASCO lab easy to follow and understand. The crystal structure in this lab was a cubic crystal structure that had metal spheres placed in a symmetric fashion. This lab also used some information and insight from Field and Cornick’s article on microwave Bragg diffraction in a model crystal lattice for the undergraduate laboratory\textsuperscript{4}. However Field and Cornick did use a different crystal structure than the one used in this lab; their lattice was one composed of metal rods.\textsuperscript{4} There is a fair amount of information regarding Bragg diffraction and Microwave optics in the American Journal of Physics and there are a few more experimental sources in Cornick’s and Field’s American Journal of Physics.\textsuperscript{4} The outline of the article is, firstly, theory will take a brief look behind the history of Bragg diffraction and the relationship between the angle of reflection and the distance between the planes. Experimental apparatus give a description of the apparatuses used in the lab; next, the lab’s procedure will discuss how the lab was performed. Following the procedure the data analysis will explain how the data was analyzed and where the error in the data came from. Lastly the discussion will compare the final results, discuss the meaning of the results, and discuss the possible improvements that could be made.
II. THEORY

Microwaves are electromagnetic waves that have wavelengths ranging from approximately 0.3 meters to 0.1 millimeters. Microwaves have a relatively short wavelength, this is ideal for studying the atomic and molecular properties of matter. The spectrum of electromagnetic waves best suited for looking at crystal structure and atomic separation distances in solids in the order of 0.1 nanometers is the X-ray spectrum. These electromagnetic waves are shot at the crystal structure, then a receiver takes the reflected wave and measures intensity of the beam at which the beam enters. The incident angle of the beam is the angle at which the electromagnetic wave enters the crystal lattice; and the reflected angle is the angle the beam makes as it is reflected off of a particle (in this lab metal spheres). The incident beam of electromagnetic waves makes an angle $\theta$ with one of the planes. The beam can be reflected from both the upper and lower plane. However, the beam reflected from the lower plane travels farther than the beam reflected from the upper plane. The effective path difference is

$$2d \sin(\theta) = n\lambda,$$

where $d$ is the distance between the two planes, $n$ is an integer determined by the order given, $\lambda$ is the wavelength of the rays, and theta is the grazing angle of the incident wave. This mathematical relationship was first discovered by W.L. Bragg and W.H. Bragg and is validly named as Braggs Law.

In this lab we are trying to find $d$, the distance between two parallel planes of the crystal lattice, by obtaining the grazing angle. The grazing angle is determined by rotating the microwave transmitter in a scanning fashion around the crystal lattice, and measuring the intensities and locating the different peaks for different integer values. So solving for the distance between planes, $d$, gives us,

$$d = \frac{n\lambda}{2\sin(\theta)}.$$ 

FIG.1 demonstrates a two dimensional reflection of an electromagnetic ray of two parallel crystalline planes separated by a distance $d$.

It is important to note that the rays entering from the left are the incident rays and the rays reflected upwards are the reflected rays. The three dimensional symmetry of the crystal
structure, as well as the constant vertical position of the microwave transmitter and receiver allows the experimental calculations to be considered in two dimensions, instead of three dimensions. In addition, the transmitter and the detector must be rotated simultaneously by equal amounts relative to the crystal to ensure that the Bragg condition holds when observing a peak. When observing a peak, Bragg’s law occurs when $\theta_{inc} = \theta_{ref} = \theta_{Bragg}$ is satisfied; where $\theta_{inc}$ is the incident angle, $\theta_{ref}$ is the reflected angle, and $\theta_{Bragg}$ is the grazing Bragg angle that is recorded in this lab.$^6$

### III. EXPERIMENTAL APPARATUS

This experiment followed the procedures found in the PASCO’s Microwave Optics Lab, experiment 12: Bragg diffraction.$^3$ For this experiment, we utilized the microwave transmitter, microwave receiver, the Goniometer, a cubic lattice, and various securing tools, meter sticks and rulers. A Goniometer is the apparatus that measures the grazing angle; and allows the transmitter to move in a scanning fashion. Alterations to the PASCO’s set up of the experiment, because a rotating table was not available. Instead the cubic crystal was secured on top of the Goniometer. The equipment was arranged as shown in FIG. 2.$^3$

The microwave transmitter was initially set 180 degrees apart from the receiver, and the meter multiplier was set at one. The grazing angle was at 90 degrees; the grazing angle is defined in FIG. 3.$^3$
IV. PROCEDURE

A standard 30 cm ruler was used to measure the actual distance between the two planes of the crystal lattice; this distance was measured from and to the centers of the parallel metal spheres. The error in this measurement was determined to be $\pm 0.001$ m; this was due to experimental uncertainty of the ruler, and the uncertainty of the location of the center of the metal spheres. The value obtained was $0.038 \pm 0.001$ m.

After setting up the experimental apparatus shown in FIG. 2, the first set of data was collected. The initial grazing angle was set at 90 degrees, and the set of planes of (100) were parallel to the incident microwave beam. The 'designations of (100), (110) and (210) are the Miller indices for these sets of planes$^3$ in the crystal lattice structure. For the next set of data, the grazing angle was initially set at 45 degrees, and the 110 planes were parallel to the incident microwave beam. The FIG.4 demonstrates the family of the planes of the crystal lattice; two sets of parallel planes are assigned different designations. The distance between the set of planes is the distance that is being determined in the experiment.$^3$

When rotating the crystal on the Goniometer one degree clockwise, it is important to
rotate the arm connecting the transmitter two degrees clockwise. Once the data is collected a graph for each of the trials was plotted; these graphs are shown the Data Analysis portion of this article.

V. DATA ANALYSIS

Before we graphed the data, the error in the initial measurements made were discussed. We had concluded that the error in the angle measurement was ± 0.5 degrees; the error in the angle measurement could have been smaller if not for the placement of the crystal lattice on the Goniometer. The placement of the crystal made the grazing angle difficult to read. We also came up with an error of ± 0.03mA error in the intensity; this is because when some of the intensity readings were made the gauge varied by plus or minus 0.03mA. FIG 5 is the set of data for the first trial, where the initial grazing angle was 90 degrees; and FIG. 6 is the set of data for the second trial, where the initial grazing angle was 45 degrees.

Once data was obtained, various intensity peaks at various angles were analyzed to determine the peak of the intensities; and to determine where and if the peaks of integer values, n=1, n=2, or n=3, occurred. In FIG. 4 the approximate angle value where the intensity peak n=1 occurred is 110 degrees; and the approximate angle value for the second intensity
FIG. 5: Plotted Data for initial grazing angle of 90 degrees

![Grazing Angle vs Intensity for Initial Angle of 90 Degrees](image)

peak of n=2 occurred at 140 degrees; these values are relative to the initial angle of 90 degrees. In FIG.5 the approximate angle value where the intensity of n=1 occurred at 67 degrees.

FIG. 6: Plotted Data for Trail 1, initial grazing angle of 45 degrees

![Grazing Angle vs Intensity for Initial Angle of 45 Degrees](image)
degrees, relative to the initial angle of 45 degrees. The Gaussian approximation is used to determine the exact angle value where the intensity peaks occurred; the angle value where the peak occurred is mean of the Gaussian Graph. The Gaussian approximation was given by,

\[ f(x) = ae^{-0.5\left(\frac{x-\mu}{\sigma}\right)^2}, \]  

where \( a \) is the amplitude of the Gaussian curve, \( \mu \) is the mean of the curve; the mean of the curve told us the angle at which the peak intensity occurred at. And \( \sigma \) is the standard distribution, the width, of the Gaussian curve. There was also error in the \( \mu \), the mean value of the Gaussian, when the data was being fitted on Gnuplot. However, in this lab, the error was still reasonable enough to carry on with the calculations. Through analysis and comparison of our data, testing different \( n \) values with our data and discussion with the instructor, Dr. Joss Ives, it was determined that for the first trial (initial \( \theta_{Bragg} = 90 \) degrees) \( n=1 \) occurred at 20.88 ± 0.50 degrees, and \( n=2 \) occurred at 49.98 ± 0.52 degrees. And for the second trial (initial \( \theta_{Bragg} = 45 \) degrees) \( n=1 \) occurred at 22.52 ± 0.63 degrees. There are errors associated with these values, they will be discussed in the Discussion of this lab. The information extracted from the Gnuplot graph, an example is FIG.7, the peak intensity for the first trial and first integer peak (\( n=1 \)).

FIG. 7: Gaussian Approximation for Trail 1, initial grazing angle of 90 degrees; \( n=1 \)

Once the means were extracted from the Gaussian plot; we used equation 2 to find the
distance between the planes. The distance between the planes, it \(d\), can be found using \(\lambda\), the wave length of the microwaves; \(n\), an integer; and \(\sin(\theta)\), where theta is the mean value of the Gaussian curves relative to the initial angle. The experimental distances between the planes was found in this experiment are in Table 1.

Experimental Values of the distances between the planes, it \(d\)

<table>
<thead>
<tr>
<th>Trial, Integer number</th>
<th>Distance, (d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial1, (n = 1)</td>
<td>0.0400 ± 0.0028 m</td>
</tr>
<tr>
<td>Trial1, (n = 2)</td>
<td>0.03723 ± 0.00024 m</td>
</tr>
<tr>
<td>Trial2, (n = 1)</td>
<td>0.0372 ± 0.0020 m</td>
</tr>
</tbody>
</table>

TABLE I:

The average of these experimental distances was found to be 0.0381 ± 0.0014 m.

VI. DISCUSSION

Looking at Table 1, the three values for the distance between the the planes coincided with one another, meaning the values agreed with in error of each other. The actual, measured, distance between the parallel planes of the crystal lattice, 0.038 ± 0.001m, coincided with the experimental average of the distance. The actual value of the distance agreed with the different trial values, shown in Table 1. The actual distance between the spheres agreeing with the experimental distances confirms the relationship given by Bragg’s Law, \(2d\sin(\theta)=n\lambda\), holds true.

It is also important to discuss that in this lab we had peaks show up that were not actual Bragg Diffraction peaks. These extra peaks could be interference from different sources around the classroom, but more likely this could be interference scattering from the microwaves bouncing off of the metallic spheres that were not in the same plane path. The way to differentiate between the actual peaks and the interfering peaks, is to plug in different integer values to see which data results coincide the best.

Some improvements that could be made on this lab is the addition of a rotating table, which was not available for this experiment. For this lab, the cubic lattice was directly secured to the Goniometer; this decreased the visibility of the angle scale on the Goniometer.
making the collection of the grazing angle data harder, increasing the relative error on the
grazing angle. Also it is important to remember that intensity is measure in milliamps,
in other words there is an extra factor of $10^{-3}$ when calculating the distance between the
planes, $d$.

In conclusion, this lab was successfully completed; this lab yielded the distance between
the parallel planes in the crystal lattice. The various results for distance, $d$, found in the
trials agreed with in error, and the measured and experimental values for distance also
agreed with one another.

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1. The Nobel Foundation, Nobelprize.org.nobelprizes.laureates (1915)
   A 88, 428-438 (1913).
3. E. Ayars, and D. Griffiths, ”The PASCO scientific 012-04630E Model WA-9314B Microwave
   Optics manual,” available from PASCO scientific, 10101 Foothils Blfv. Roseville, CA 95747-7100
4. M.T. Cornik and S.B. Field, ”Microwave Bragg diffraction in a model crystal lattice for the
5. R.A. Serway and J.W. Jewett, Physics for Scientists and Engineers with Modern Physics, Sixth
   Edition, Brooks/Cole- Thomson Learning, 10 Davis Drive, Belmont, CA 94002, USA, 1080-1225
   (2004).
6. J.C. Amato and R.E. Williams, ”Rotating Crystal Microwave Bragg diffraction apparatus,”Am.