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Experiment 2: Observation of Bragg Diffraction in Styrofoam Model

Kaimi Kahihikolo

Abstract

Bragg's Diffraction is a principle of light which describes the scattering of light within a crystalline structure. Utilizing a model, comprised of Styrofoam and metal ball bearings, and a microwave source (and detector), Bragg's Diffraction is successfully observed. Using this principle, the plane spacing within the structure was determined to be $0.038 \pm 0.003\,[m]$ and $0.038 \pm 0.001\,[m]$, which both agree with the separation directly measured with calipers $(0.038 \pm 0.001\,[m])$—within 1σ certainty.

1 Introduction

Bragg Diffraction is defined as the process that occurs when coherent light scatters off of planes in a crystal lattice structure. Bragg Diffraction is an important phenomenon that is used to understand atomic and molecular structures though x-ray crystallography.

The goal of this experiment is to observe Bragg diffraction and utilize this effect to determine the plane spacing, a, of the Styrofoam model. This will be done by analyzing the planes (1,0,0) and (2,1,0)—see Section Miller Indices for explanation—which will be referred to as plane A and B, respectively.

2 Theory

Figure 1 illustrates the geometry of Bragg diffraction, which occurs when rays of light reflect off of parallel planes of atoms, in a crystalline lattice structure, is equal to an integer multiple of the wavelength of the incident light. A result of this is the superposition of the reflected waves. The path difference of the parallel light rays, as a result of refraction, is dependent on

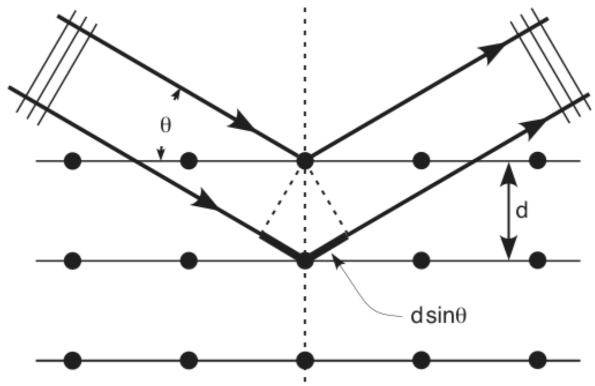

Figure 1: Bragg Diffraction Geometry
(https://commons.wikimedia.org/wiki/File:Bragg_diffraction.png)

the incident angle from the source. When the angles meet the Bragg condition, constructive interference occurs. On the contrary, destructive interference occurs at angles that meet a half integer requirement.

$$n\lambda = 2dsin(\theta) \Rightarrow \theta = \arcsin(n\lambda/2d) \;\; (\forall\, n \in \mathbb{Z}) \tag{1}$$

where λ is the wavelength, θ is the angle of incident light (with respect to the crystal plane), and d is the separation, see equation 2.

See Appendix A for the derivation of Bragg's equation (equation 1) to second order using a taylor expansion.

2.1 Miller Indices

To describe the structure of a crystal, Miller Indices are utilized (h,k,l)—where (h,k,l) are integer values. These indices can be thought of as a Cartesian (x,y,z) coordinate system. Using equation 2, one can determine the distance between two planes (h,k,l).

$$d_{h\,k\,l} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{2}$$

3 Procedure

The apparatus utilizes a microwave source with a frequency of $f = (1.05 \pm 0.01) \times 10^{10}\,[Hz]$ and a detector that measure current in $[mA]$. The model consists of a Styrofoam cube with a plane A spacing, a_{theo}, of $3.8 \pm 0.1\,[cm]$. The microwave source is located approximately $50\,[cm]$ from the Styrofoam model. The apparatus also utilizes a goniometer to measure the diffraction at resultant angles as a function of the incident angle.

1. Measure lattice constant with calipers and its associated error
2. Align goniometer arms parallel to each other. Similarly, align cube model such that plane A is parallel with the arms.
3. Record the current from the receiver (also note its error and scale value).
4. Rotate cube and the receiving arm clockwise 5°, and record its current and the angle; repeat this step until a grazing angle (θ_g) of 10°.
5. While $\theta_g = 10 \rightarrow 35°$, sample at 1°increments, then return to 5°increments as before.
6. Reset apparatus with the cube oriented such that plane B is parallel with the goniometer arms.
7. Sample the current in increments of 5°until a grazing angle of 40°, then sample at 1°increments.
8. Plot the current against grazing angle. Locate the angles with central maxima and their associated errors.
9. Using equation 1, determine the layer separation, d, for each plane and its error.
10. Using these values, determine a_{exp} using equations 4 and 5 and its error. Determine if the experimental value agrees with the theoretical (measured with calipers).

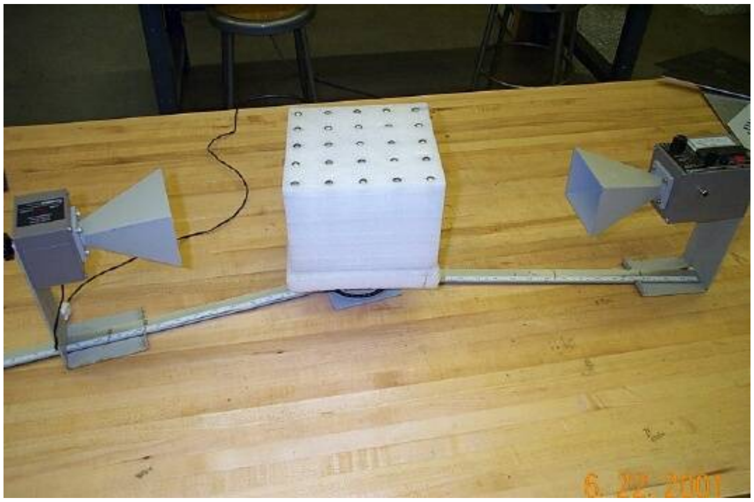

Figure 2: Picture of apparatus (http://www.physics.rutgers.edu/ugrad/labs/bragg)

4 Data

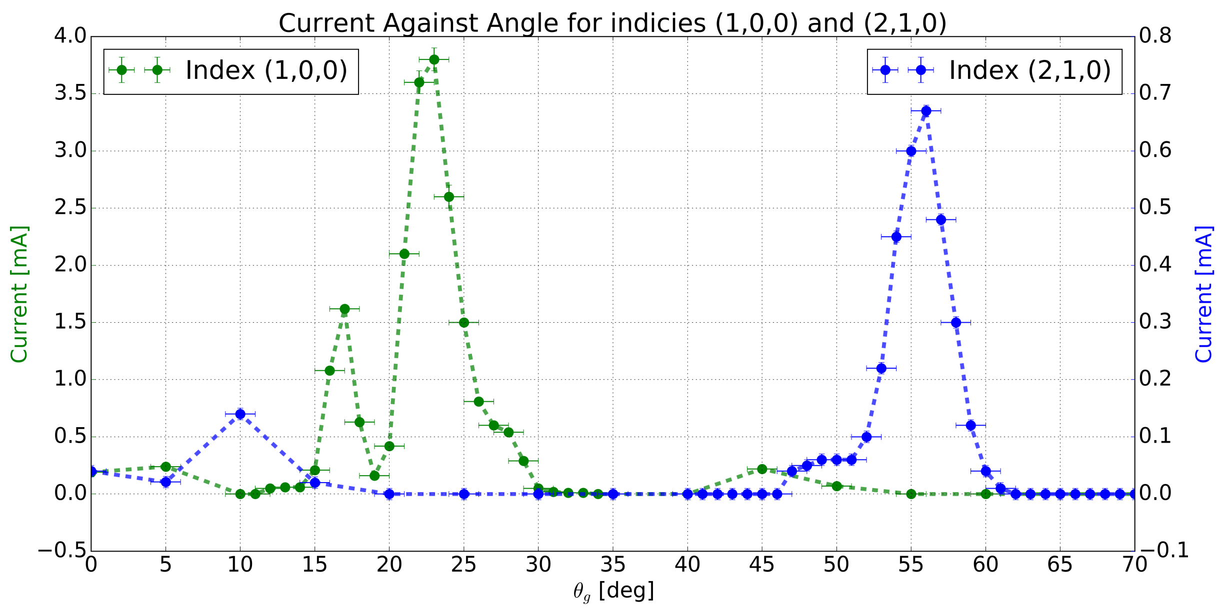

Figure 3: Measurements taken for planes A and B.
(1,0,0) Peaks [deg] : 3.0 ± 1.0, 17.0 ± 0.5, 23.0 ± 1.0, 46.0 ± 1.0.
(2,1,0) Peaks [deg]: 0.0 ± 2.0, 10.0 ± 0.5, 56.0 ± 1.0.

5 Results

5.1 Theoretical Calculations

By utilizing the wavelength of the source, the theoretical angles that show Bragg's condition can be determined with equation 1 and 3.

$$\lambda = \frac{c}{f} = \frac{299,792,458\,[m\,s^{-1}]}{(1.05 \pm 0.01) \times 10^{10}\,[Hz]} = 2.86 \pm 0.03\,[m] \tag{3}$$

Using the Miller Indices, the separation can be expressed in terms of the lattice constant, a, where $a_{theo} = 3.8 \pm 0.1\,[cm]$.

$$d_{100} = \frac{a}{\sqrt{1^2 + 0^2 + 0^2}} = a \pm \delta a \tag{4}$$

$$d_{210} = \frac{a}{\sqrt{2^2 + 1^2 + 0^2}} = \frac{a \pm \delta a}{\sqrt{5}} \tag{5}$$

Using equation 1, the following angles, in degrees, that satisfy Bragg's Condition are:

$$\theta_{100} = 22.1 \pm 0.7,\ 48.7 \pm 1.8$$

$$\theta_{210} = 57.1 \pm 2.5$$

where the errors are calculate via Python with the standard propagation of error procedure.

5.2 Experimental Results

Using figure 3, the angles, in degrees, with central maxima are:

$$\theta_{100_{exp}} = 3.0 \pm 1.0,\ 17.0 \pm 0.5,\ 23.0 \pm 1.0,\ 46.0 \pm 1.0$$
$$\theta_{210_{exp}} = 0.0 \pm 2.0,\ 10.0 \pm 0.5,\ 56.0 \pm 1.0$$

It can be seen that some of the experimental angles agree with the theoretical results,

$$\%_{100} = \frac{\theta_{100_{theo}} - \theta_{100_{exp}}}{\theta_{theo}} \times 100\% = 0.3\%, 5.6\%$$
$$\%_{210} = 2.9\%$$

Now, using the angles associated with the central maximum in each plane, the separation can be calculated using equation 1,

$$d_{100_{exp}} = \frac{\lambda}{2 \times sin(\theta_{100_{exp}})} \simeq 0.038 \pm 0.003\,[m] \tag{6}$$
$$d_{210_{exp}} = \frac{\lambda}{2 \times sin(\theta_{210_{exp}})} \simeq 0.0173 \pm 0.0004\,[m] \tag{7}$$

Recall equations 4 and 5, therefore...

$$a_{100_{exp}} = d_{100_{exp}} \simeq 0.038 \pm 0.003\,[m] \tag{8}$$

$$a_{210_{exp}} = d_{210_{exp}} \times \sqrt{5} \simeq 0.038 \pm 0.001\,[m] \tag{9}$$

6 Discussion

It can be seen from the results that the theoretical plane spacing, $a_{theo} = 3.8 \pm 0.1\,[cm]$, measured with the calipers does agree with the results achieved through the experiment. In the (1,0,0) plane, the separation was determined to be $0.038 \pm 0.003\,[m]$ which has a z-score of 0.03σ. For the (2,1,0) plane, the separation is $0.038 \pm 0.001\,[m]$, which has an associated z-score of 0.73σ. Overall the results are highly accurate, well within 1σ certainty. Due to this accurate, it can be can confirmed that Bragg diffraction has been observed.

An interesting effect noticed while conducting experiment is that drifting zero detected by the receiver may be a possible source of error—specifically a positive error. Also, it can be seen in Figure 3 that others peaks can be observed besides those predicted by Bragg's Law, 1. Those peaks may be attributed to 2nd order diffraction occurring between the metal balls within the model.

7 Conclusion

Bragg's Diffraction was successfully observed within the Styrofoam toy model. Using this effect, the plane spacing, a, was determined to be $0.038 \pm 0.003\,[m]$ in plane A, which is within 1σ of the plane spacing directly measured with the calipers ($0.038 \pm 0.001\,[m]$). When repeated with a different plane (plane B), a was determined to be $0.038 \pm 0.001\,[m]$, which also agrees with the separation directly measure with calipers.

8 Appendix A

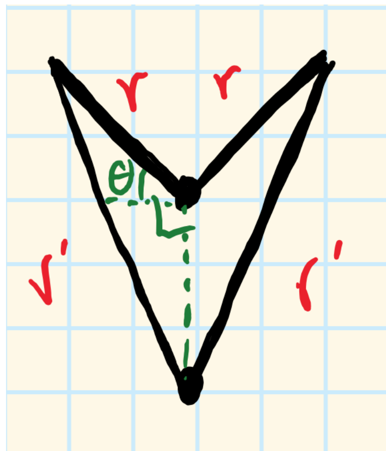

Figure 4: Geometry used for derivation, where the distance between "atoms" is d

$$(r')^2 = d^2 + r^2 - 2rdcos(\theta + 90°) = d^2 + r^2 + 2rdsin\theta$$

$$r' = \sqrt{d^2 + r^2 + 2rdsin\theta} = \sqrt{r^2\left(\frac{d}{r}\right)^2 + 1 + \frac{2dsin\theta}{r}}$$

$$= r\sqrt{1 + \left(\frac{d}{r}\right)^2 + \frac{2dsin\theta}{r}}$$

Recall: $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2$, for $x << 1$

$$\Rightarrow r' = r\left[1 + \frac{1}{2}\left(\left(\frac{d}{r}\right)^2 + \frac{2dsin\theta}{r}\right) - \frac{1}{8}\left(\left(\frac{d}{r}\right)^2 + \frac{2dsin\theta}{r}\right)\right] \approx \frac{1}{2}\frac{d^2}{r}cos^2\theta + dsin\theta + r$$

$$\Rightarrow r - r' = \frac{1}{2}\frac{d^2}{r}cos^2\theta + dsin\theta$$