Microwave Bragg diffraction in a model crystal lattice for the undergraduate laboratory

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We describe an undergraduate laboratory experiment in which Bragg diffraction is studied using microwave diffraction from a two-dimensional crystal consisting of a square lattice of metal rods. This apparatus demonstrates the fundamental ideas of the Bragg theory of crystal diffraction using a macroscopic model. Thus, the geometrical relations between the crystal planes and the incoming and scattered wave directions are clearly visible. A key element of the apparatus is a computer interface that allows diffracted intensity measurements at all orientations of crystal and detector. No a priori assumptions need be made concerning the relation between the incident and refracted angles. We also present results of computer simulations of the scattering from our crystal. These simulations have been useful in understanding the differences between the simple Bragg theory and the results from our experiment on a small crystal with finite source and detector distances. © 2004 American Association of Physics Teachers.

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I. INTRODUCTION

W. L. Bragg and W. H. Bragg were the first to use data from diffraction experiments to deduce the structure of an atomic crystal. In the undergraduate laboratory, Bragg diffraction often is demonstrated using the diffraction of x rays or electrons from a crystal. To the student, however, such experiments often appear quite abstract, because both the atomic structure of the crystal and the wave itself are invisible to the eye. To supplement these atomic diffraction experiments, we have made use of a macroscopic model of Bragg diffraction, in which microwaves are scattered off a crystal with a lattice spacing of order centimeters. The students can directly correlate maxima in the scattered intensity with the orientation of the microwave beam and the crystal plane, thus gaining insight into the geometrical relationships imposed by the Bragg conditions.

Several microwave Bragg experiments have been previously reported. Metallic scatterers such as disks, brads, or metal balls are spaced in a three-dimensional lattice, the scatters being spaced by insulating rods, strings, or styrofoam. The data consist of intensity versus angle plots. For an arbitrary orientation of crystal and detector there will in general be no scattered intensity. Thus Murray used a special table designed so that as the crystal rotates through an angle $\theta$, the microwave receiver rotates through an angle $2\theta$, automatically enforcing the Bragg condition [see Eq. (1)] that the incident and reflected angles must be equal. Allen used the simpler expedient of setting the crystal at an angle at which strong scattering was expected, and then rotating the detector to search for an intensity maximum.

Our apparatus differs from these earlier ones in two ways. First, although the crystals described above are three dimensional, the scattering is effectively two dimensional. This is because the detector is swept in a circle whose plane is perpendicular to an axis of crystal symmetry. Thus the existence of horizontal planes of atoms plays no role in the observed diffraction pattern. Because of this, we have simply replaced the complex three-dimensional crystal with a two-dimensional one made up of vertical rods. Second, the use of $\theta, 2\theta$ tables or other schemes to make certain that intensity peaks were observed seems to us to be pedagogically unsound. We would prefer that students discover experimentally the fact that scattering only occurs for such orientations where the incident and reflected angles are equal, and not have this geometry imposed by the apparatus. To do this, data must be taken at all possible angles of crystal and detector, a requirement which can only be reasonably met by using a computer to aid in data taking. In our instrument both the intensity and the angle of the crystal are automatically recorded by a computer.

II. EXPERIMENTAL APPARATUS

As shown in Fig. 1, the experimental apparatus consists of a fixed microwave source, a rotatable microwave detector, and a model crystal. The source and detector are commercially available units. The 10 mW, 10.52 GHz source (wavelength $\lambda = 2.85$ cm) is polarized parallel to the rods, and sits on the lab table about 1 m from the center of the apparatus. The detector is mounted 1 m from the center of the apparatus on wooden arm A. This arm is rigidly attached to turntable B; the arm and turntable are free to rotate around pivot C which is attached to the fixed base D. As shown in the inset to Fig. 1, the pivot consists of a 3/8 in. bolt with a 3/8 in. extension piece soldered to its top. (The base sits on small feet so that the pivot’s nut clears the table.) Protractor E is used to measure the angle of the detector arm. This protractor is prevented from rotating by pin F. The model crystal is constructed from 64 aluminum rods G placed on an 8 x 8 grid with a lattice spacing $d = 3.70$ cm. Each rod is 11.5 cm long and has a diameter of 1/16 in. The rods are fitted into holes drilled into two acrylic plates H that are held rigidly apart by acrylic rods at the plates’ corners. The entire crystal can be rotated by hand about an axis through its center and parallel to the rods. A computer is used to measure the crystal angle by reading the voltage from potentiometer J, which is attached to boss K with setscrews. The potentiometer is held fixed by arm L.

The several angles used in the experiment are defined in Fig. 2. We define the crystal rotation angle $\alpha$ as that between the crystal’s x axis and the direction of propagation of the
microwave beam from the fixed source. The detector is free to rotate in a large circle around the crystal’s center; this angle is defined in Fig. 2 as $\beta$.

An important feature of this apparatus is that it allows a measurement of the diffracted microwave intensity at every combination of crystal and detector angle. To take this large amount of data efficiently, it is necessary to use a computer interface. The crystal angle $\alpha$ is directly measured by the computer as follows. A potentiometer, attached to the crystal axis, has 5 V applied across its two fixed terminals. The moving terminal then reports a 0 to 5 V reading which is proportional to the angle $\alpha$. This voltage is then read by an analog-to-digital converter (ADC) board within the Macintosh computer. The microwave intensity measured by the detector is also recorded by the ADC board. It would also be possible to measure the crystal angle using a digital optical encoder. Unlike potentiometers, such encoders can be rotated through arbitrarily large angles. Students tend to rotate the crystal past the potentiometer’s stop, wrenching its shaft.

Intensity maps are obtained using a simple LabView interface. First, the potentiometer is calibrated by setting the crystal to $\alpha = 0^\circ$, making an angle reading using the ADC, and then repeating the procedure with the crystal at $\alpha = 90^\circ$. These two ADC readings can then be used to map any ADC reading into an angle $\alpha$. Next, the detector is placed by hand at an initial angle near $20^\circ$; at smaller angles the detector is swamped by the direct beam from the source. The crystal angle $\alpha$ is then set to slightly less than $0^\circ$. A Go button on the LabView interface is pressed, and the operator begins smoothly turning the crystal through and slightly past $90^\circ$. During this time, the ADC reads the potentiometer and, simultaneously, the detector output by taking 500 data points evenly spaced over five seconds. A LabView algorithm interpolates this large data set to output 180 intensity points, spaced every 1/2 degree in $\alpha$. Because $\alpha$ is read directly by the ADC along with the intensity data, this interpolation scheme means that the operator need not turn the crystal at a particularly constant rate. Further, the algorithm uses the known ADC values at $0^\circ$ and $90^\circ$ to find precisely when to start and end a sweep of $\alpha$. Thus $\alpha$ need not be precisely set to $0^\circ$ at the beginning or to $90^\circ$ at the end of a run. Indeed,
the crystal may be rotated either from 0° to 90°, or from 90° to 0°, even on successive rotations, saving quite a bit of time. This procedure is repeated for many different detector angles \( \beta \). A preliminary run might use 5° increments in \( \beta \) and a final run 2° increments.

We show the results of such a run in Fig. 3(a), where we plot the diffracted microwave intensity as a function of detector angle \( \beta \) and crystal angle \( \alpha \). There are clear concentrated regions of high microwave intensity. Because \( \alpha \) and \( \beta \) are not angles typically discussed in textbook treatments of Bragg diffraction, we must understand how the observed intensity pattern relates to the standard case.

### III. DATA ANALYSIS

In Bragg diffraction, we consider a plane wave incident at an angle \( \theta_i \), measured from the surface of a crystal plane, and reflecting off at angle \( \theta_r \) (see Fig. 2). Each plane is defined by its Miller indices, which are the smallest integers \( (k \ell m) \) such that the normal to the plane is \( k \hat{x} + \ell \hat{y} \). Here, \( \hat{x} \) and \( \hat{y} \) are unit vectors in the \( x \) and \( y \) directions, respectively. Because there are two oppositely directed normals to a given plane, a choice must be made. We have taken the normal that points down for a plane parallel to the x axis. The normals for other planes are this normal, rotated by the same angle \(< 90°\) by which the other plane is rotated from the x axis. With this convention, the Miller indices of a plane parallel to the x axis are \((0 \bar{1} \bar{1})\), and the plane at 45° between the x and \( -y \) axes in Fig. 2 is the \((\bar{1} \bar{1} \bar{1})\) plane, where a bar over an index indicates a negative value.

The Bragg diffraction conditions are that the incident angle equals the reflected angle, or

\[
\theta_i = \theta_r = \theta, \tag{1}
\]

and that

\[
2d_k \ell \sin(\theta) = n \lambda. \tag{2}
\]

Here, \( d_k \ell \) is the distance between \((k \ell m)\) crystal planes, \( \lambda \) is the wavelength of the incident wave, and the integer \( n \) is called the order of the diffraction. As in Fig. 2, we may define a crystal plane by the counterclockwise angle \( \phi \) it makes with the x axis of the crystal. Thus, for example, the \((\bar{1} \bar{1} \bar{1})\) plane shown has \( \phi = -45° \). We can then deduce the following relations between the various angles. We note that

\[
\beta = \theta_i + \theta_r = 2 \theta, \tag{3}
\]

where we have used the first Bragg condition, Eq. (1); we have further that

\[
\theta_i = \theta = \alpha + \phi. \tag{4}
\]

If we combine Eq. (4) with Eq. (2), we find

\[
\beta = 2 \arcsin \left( \frac{n \lambda}{2d} \right), \tag{5}
\]

and

\[
\alpha = 2 \beta - \phi. \tag{6}
\]

Equations (5) and (6) then give us the positions of the expected Bragg peaks in the two angles \( \alpha \) and \( \beta \).

We can now calculate the expected peak positions for our crystal. We first choose a crystal plane by giving its indices \((k \ell m)\). We also choose an order \( n \). The angle \( \phi \) is then given by \( \phi = -\arctan(k/\ell) \), and the distance \( d_k \ell \) between two such planes is given as \( d_{k \ell} = d / \sqrt{k^2 + \ell^2} \). We may then calculate \( \alpha \) and \( \beta \) from Eqs. (5) and (6). For most choices of \( k \), \( \ell \), and \( n \), either the resultant angle \( \alpha \) is outside the range of 0° to 90° studied, \( \beta \) exceeds 180°, or the argument of the arcsine in Eq. (5) exceeds 1 so that the second Bragg condition cannot be satisfied. In fact, there are only five combinations of \( k \), \( \ell \), and \( n \) that lead to predicted peaks in the observed range of \( \alpha \). These are shown in Table I. In Fig. 3(a) we plot the positions of these predicted Bragg peaks (open circles) on the measured data. There is general agreement between the data and the theoretical points; in particular, experimentally there are clearly five spots in about the correct location (with one spot “folded” at 90° back to near 0°). However, the peaks in the measured intensity are quite broad and asymmetric, espe-

### Table I. Values of \( \alpha \) and \( \beta \) predicted from the Bragg conditions, Eqs. (5) and (6).

<table>
<thead>
<tr>
<th>( k \ell )</th>
<th>( n )</th>
<th>( d_{k \ell} ) (cm)</th>
<th>( \phi ) (°)</th>
<th>( \beta ) (°)</th>
<th>( \alpha ) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0 \bar{1} \bar{1}))</td>
<td>1</td>
<td>3.70</td>
<td>0.0</td>
<td>45.3</td>
<td>22.7</td>
</tr>
<tr>
<td>((0 \bar{1} \bar{1}))</td>
<td>2</td>
<td>3.70</td>
<td>0.0</td>
<td>100.8</td>
<td>50.4</td>
</tr>
<tr>
<td>((\bar{1} \bar{1} \bar{1}))</td>
<td>1</td>
<td>2.62</td>
<td>-45.0</td>
<td>66.0</td>
<td>78.0</td>
</tr>
<tr>
<td>((\bar{1} 2 \bar{1}))</td>
<td>1</td>
<td>1.65</td>
<td>-26.6</td>
<td>118.9</td>
<td>86.0</td>
</tr>
<tr>
<td>((1 \bar{2} \bar{1}))</td>
<td>1</td>
<td>1.65</td>
<td>26.6</td>
<td>118.9</td>
<td>32.9</td>
</tr>
</tbody>
</table>

Fig. 3. (a) Microwave intensity versus crystal angle \( \alpha \) and detector angle \( \beta \). Dark areas correspond to higher intensity. Reasonably well-defined dark spots correspond to Bragg diffraction peaks. Data were taken every degree in \( \beta \). Open circles are predicted peak positions from Eqs. (5) and (6). (b) Computer simulation of the 8x8 crystal, including multiple scattering.
A reciprocal lattice point rotates as well. Thus in Fig. 4 the (01) lattice point rotates by an angle \( \alpha = 22.7^\circ \) before intersecting the circle at point \( a \). Geometrically, \( \beta \) is the angle between \( \mathbf{k} \) and \( \mathbf{k}' \) as shown; we can measure this angle to be \( 45.3^\circ \), consistent with Table I. As the crystal is further rotated, other lattice points intersect the circle at points \( b \), \( c \), and \( d \), defining new values of \( \alpha \) and \( \beta \). Note that two lattice points hit the circle at \( d \), implying two Bragg peaks with the same \( \beta \) but different \( \alpha \)'s, as observed. Five of the spots inside the circle also intersect it, but lead to \( \mathbf{k}' \) vectors pointing in the positive half of reciprocal space. The detector would have to moved to the other side of the apparatus to observe these spots. Finally, we can see that the indices of the five reciprocal lattice points that intersect the Ewald circle correspond to the Miller indices of the five planes used in the Bragg analysis in Table I, reflecting the fundamental fact that any reciprocal lattice vector \( \mathbf{G}_{k\ell} \) is perpendicular to the Bragg plane with Miller indices \( (k\ell) \).

IV. COMPUTER SIMULATIONS

We have seen that there are systematic differences between our data and the predictions of the Bragg theory. Such differences are expected: the Bragg theory holds for perfect plane waves incident on an infinite crystal with weak scattering, while experimentally the source and detector are relatively close to the finite-sized crystal, and multiple scattering may be important. To investigate these issues, we have performed computer simulations of the scattering off a finite crystal. The source is approximated as an infinite line source emitting cylindrical waves. Each infinitely long rod emits a cylindrical wave according to the amplitude and phase of the incident wave at that rod’s position. The scattered amplitudes from all rods are summed at the detector position and squared to obtain the intensity.

We have performed simulations with the incident wave at each rod being either the incident plane wave alone (single scattering), or the truncated sum of the plane wave and reflected waves from the other rods (multiple scattering). For the multiple scattering case, we have used the analytically derived scattering cross section valid for the case where \( \lambda \gg a \), where \( a \) is the rod diameter. The results of such a simulation are shown in Fig. 3(b) for the case of multiple scattering. The single scattering results are qualitatively similar. The simulations match the data quite well. In particular, the diagonal elongation of the spots is reproduced, and there are even hints of some matching substructure. The simulations further show that the spot elongation is mostly an effect of the finite crystal size, and does not vanish if the source and detector are far removed.

These simulations also reveal the origin of the overall shift between the expected Bragg spots [circles, Fig. 3(a)] and the recorded intensity data. In a simulation with only single scattering, the centers of the simulated spots coincide closely with the theoretical Bragg spots. This agreement is counter to the observed data. When we use multiple scattering, however, the simulated spots become very near to the observed spots, as can be seen in Fig. 3. Apparently multiple scattering leads to a net shift of the maxima from their expected positions. A simple explanation shows why this occurs. If scattering is strong, then the scattering is weighted toward the side of the crystal nearest the source. The far side of the crystal simply receives less of the wave to scatter. If we make the crudest approximation that only the right half of the crystal in Fig. 2 was involved in scattering, then this half-crystal would be centered not at the origin, but roughly two pins to the right of the origin. Now suppose the half crystal and the detector were correctly oriented for a Bragg maximum. Because the center of the crystal has moved to the
right, the detector will also have to be moved somewhat to
the right to detect the maximum—that is, the detector will
need a larger value of $\beta$ to be at the maximum. This is what
is observed in Fig. 3(a).

This experiment has been found quite helpful in increasing
our students’ understanding of Bragg diffraction. A particular
strength of the experiment is how it allows the students to
directly visualize the crystal planes, and the planes’ geo-
métrical relationship to the incident and reflected wave di-
rections when at a Bragg peak. When the students then go on
to investigate, say, electron diffraction, the physical meaning
of the Bragg conditions has a much firmer intuitive basis.


2R. G. Marcley, “Apparatus drawing project #6: Bragg diffraction experi-

3J. J. Connelly, Jr., “Simply constructed atomic stacking models for micro-

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9R. W. P. King and T. T. Wu, The Scattering and Diffraction of Waves

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POIGNANCY IN EINSTEIN’S DESTINY

And surely the poignancy in Einstein’s destiny welled from disappointments deeper than the
drawing off of physical interest from relativity into quanta? Surely the very generality of his
liberation, rendering the perfectly benign perfectly irrelevant to the vast impersonality of nature,
invested his inner freedom and security with the loneliness of a Greek tragedy, one inhering in the
necessities of things rather than (like Galileo’s) in the characters of men.

Submitted by Gary E. Bowman.