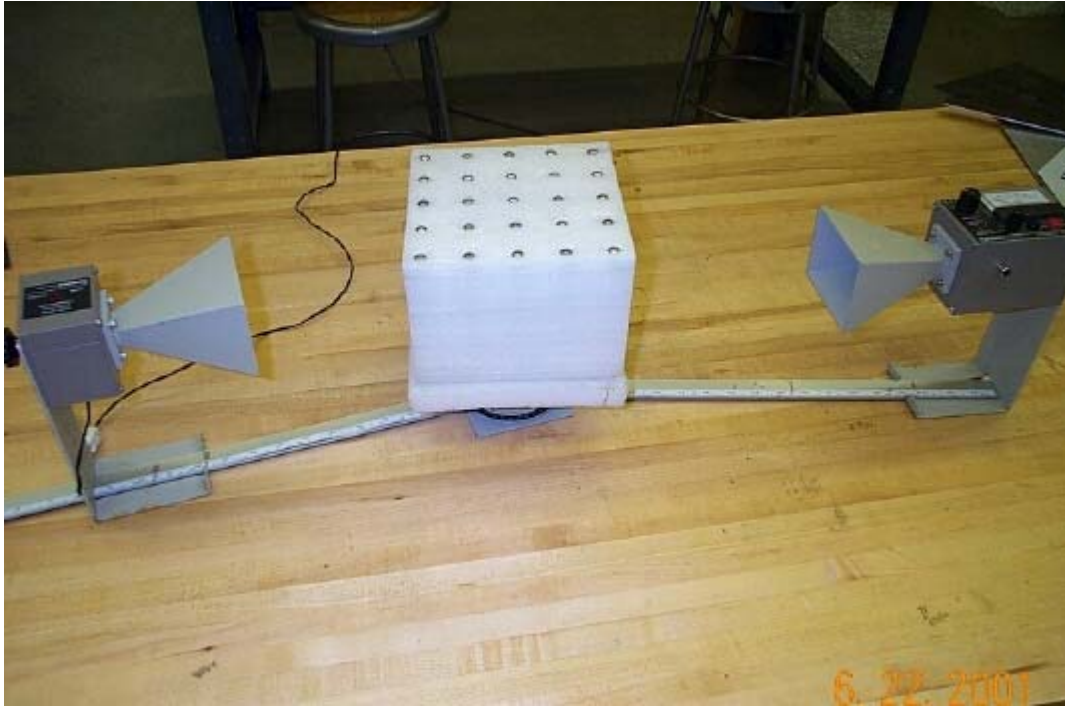


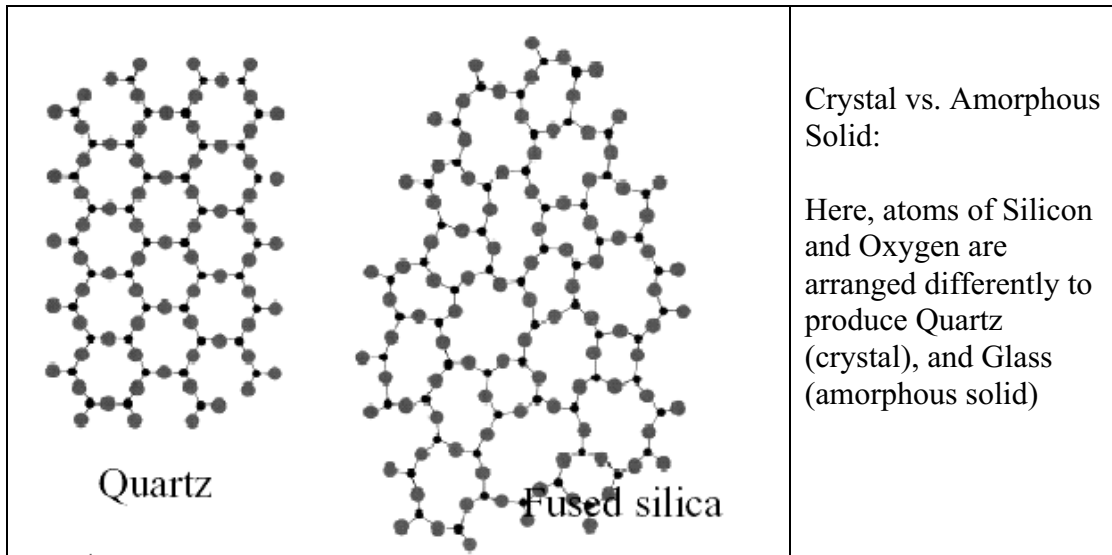
Probing Atomic Crystals: Bragg Diffraction



OBJECTIVE: To learn how scientists probe the structure of solids, using a scaled-up version of X-ray Diffraction.

APPARATUS: Steel ball "crystal", microwave transmitter & receiver, goniometer (angle measuring device), various stands & holders, meter stick

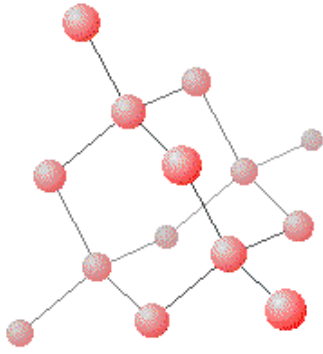
INTRODUCTION: You've heard the term "crystal" before; what exactly is it? A *crystal* is a fairly simple pattern of atoms or molecules that is repeated throughout a macroscopic solid. A crystal forms naturally when a liquid at high temperature is cooled slowly to give the atoms or molecules time to arrange themselves in a regular array. It is matter having arranged itself with maximum number of bonds and the minimum potential energy possible, and it exhibits long-range order. A single crystal can fill your hand, or can even be larger. If the high-temperature liquid is cooled so rapidly that its internal energy is taken away before matter can order itself into arrays, an *amorphous solid* results. Glass is such a material. Because of its ordered structure, a crystal will be harder and more rigid than an amorphous solid made from the same liquid.



How are the atoms arranged in a crystal? How far apart are they? You may recall that you were able to gather similar information about the structure shiny, colorful diffraction grating that you used in the *Light Wave Interference & Diffraction* experiment. Specifically, you determined the size of the grating slits and their orientation (horizontal or vertical). What about using an atomic crystal as a three-dimensional diffraction grating? This was proposed by M. Laue in 1912 and performed by W.L & W.H Bragg (father & son) the same year. Father and son Bragg were jointly awarded the Nobel Prize in 1915 for their work.

Could we shine a laser through a crystal to produce those cool interference patterns we got a few labs ago? That might work if the wavelength of light used was comparable (within an order of magnitude or so) to the spacing of the lattice (recall that laser light, $\sim 10^{-7}$ m in wavelength, was projected onto small slits of a diffraction slide, $\sim 10^{-6}$ m apart. In crystals, however, the spacing is much smaller ($\sim 10^{-10}$ m) and would require light of a much smaller wavelength. X-rays, discovered by W. Roentgen in 1895, fit the bill. In this lab however, due largely to safety concerns, we will not use X-rays and will instead use microwaves to study a very large "crystal" made of steel balls packed in foam. Here the geometry of Bragg's law remains unchanged; only the wavelength and spacing have been scaled up by a factor of 10^9 (one billion).

Bragg diffraction (diffraction via reflection) and X-ray crystal diffraction (diffraction via refraction) are widely used for determining structures of very small but ordered things. In fact, it was Rosalind Franklin, a crystallographer, who provided James Watson and Francis Crick some very valuable data and interpretations thereof that led them to the monumental discovery of the structure of DNA, the double helix.



Diamond crystal (Carbon atoms)

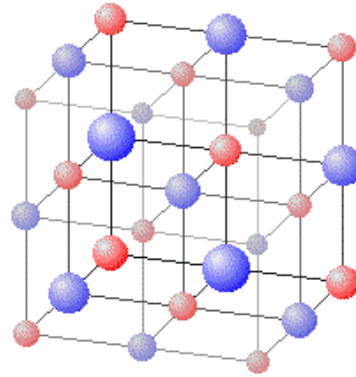


Table Salt crystal (Na and Cl atoms)

NOTE: You may be worried about being exposed to microwaves in this experiment. The output power of the transmitter is 15 mW (15×10^{-3} Watts), which is about five orders of magnitude (0.001 %) less than the power of your microwave oven at home. More importantly, the 10.5 GHz frequency used here is higher than the 2.45 GHz used in your oven, a frequency selected because it is the resonant frequency of the water molecule's rotational mode (recall the Forced Harmonic Oscillator lab). Hence the water molecules of your body do not absorb microwave radiation of this frequency.

Simple Reflection

Here you will confirm the law of reflection for microwaves incident upon a metal plate. Having the angles of incidence and reflection equal is a requirement for Bragg Diffraction to occur. Since you should be familiar with most of the equipment from last semester's *Microwave Optics: Refraction and Polarization* lab, we will dispense with a detailed apparatus description here.

PROCEDURE

1. Position the two arms of the goniometer such that they form a "V", as in the diagram on the right.
2. Position both receiver and transmitter about 10 inches from the fulcrum (center) of the goniometer). Place a mount with a hole in the base in the center of goniometer and magnetically attach a broad flat aluminum plate there. It will serve as the incident surface.



3. One goniometer arm (transmitter) is fixed at zero degrees; the other (moveable) arm will indicate angle with respect to the fixed arm. The angle of the plate can be read from the small tab or notch indicator oriented 90 degrees from the plane of incidence. Turn on the transmitter and receivers – plug in the AC adapter into the transmitter and rotate the knob on the top of the receiver. Set the sensitivity of the receiver to 30X. Rotate the base of the incident plane until you get a maximum and note down the transmitter, receiver and plate angles. Repeat this for two more sets of angles. Does the law of reflection hold for microwaves incident upon a metal plate?



Notch or Tab

Record values below, remembering that angles of incidence and reflection are measured from the line perpendicular to the plate, which is 90° away from the plate angle. Disconnect the AC adapter from the Transmitter and turn off the Receiver.

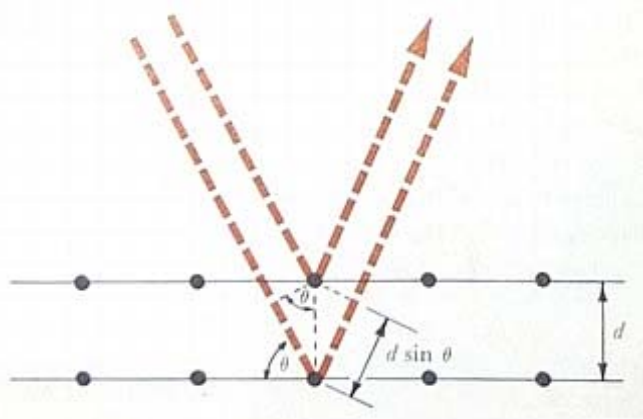
Transmitter Angle	Receiver Angle	Plate Angle	Angle of Incidence	Angle of Reflection

Bragg Diffraction

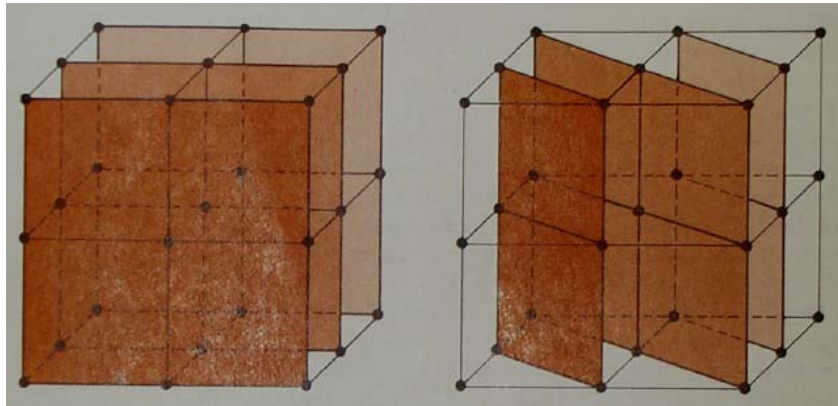
Now we will replace the metal plate with a "crystal". In addition to the requiring the angles of incidence and reflection to be equal, Bragg Diffraction also requires that waves from different **Bragg planes** interfere constructively, as described on the next page.

Look at side of the crystal block with exposed steel balls. There are similar layers of balls underneath, with constant spacing between the layers. The layer of exposed balls constitutes a *Bragg plane*, a plane from which the incident microwave is reflected. This reflected wave interferes with waves reflected from **other** Bragg planes oriented in the same direction. Examine the diagram on the right – two such waves will interfere constructively if the path difference is equal to an integer number of wavelengths:

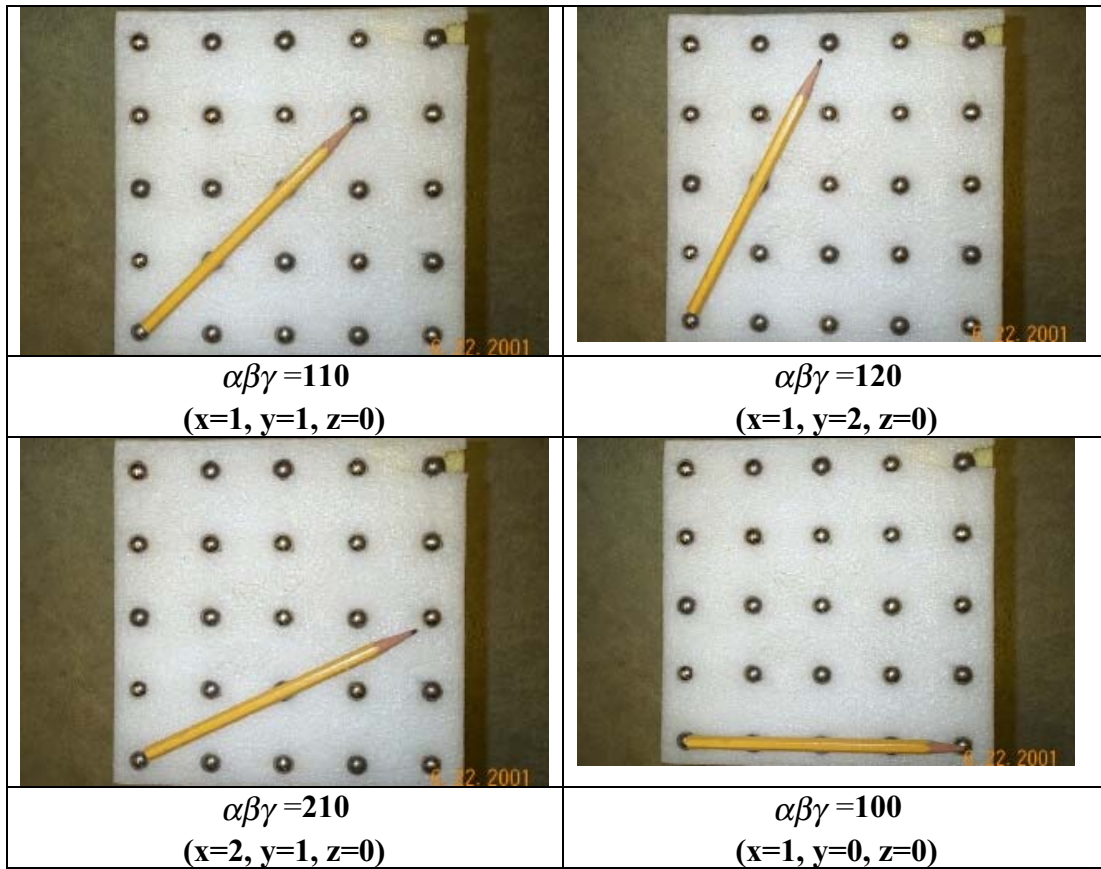
$$2d \sin \theta = m\lambda$$



You will therefore see maxima at the **grazing angles** given by the above equation, with the grazing angle measured between the incident wave and the Bragg plane being investigated. "Seeing maxima" means having the receiver detect a high meter reading at a particular angle. There are more planes to consider other than the layer of balls that you see and the parallel planes underneath it – consider this diagram of a table salt (NaCl) crystal:



Notice that depending on which atoms you group together, you can have many such Bragg planes which will have different values of d , the distance between successive planes. We use three quantities - $\alpha\beta\gamma$, known as **Miller Indices**, to define the planes. $\alpha\beta\gamma$ can be thought of as the number of steps in x,y and z to reach the next atom in the same Bragg plane. In the following pictures, the pencil represents a portion of a line on the Bragg plane that is perpendicular to the plane of the paper:



Note that the above planes all have their normal (perpendicular) in the plane of the paper (no z-component). Here is a Bragg plane that has a z-component; its designation is **111**:

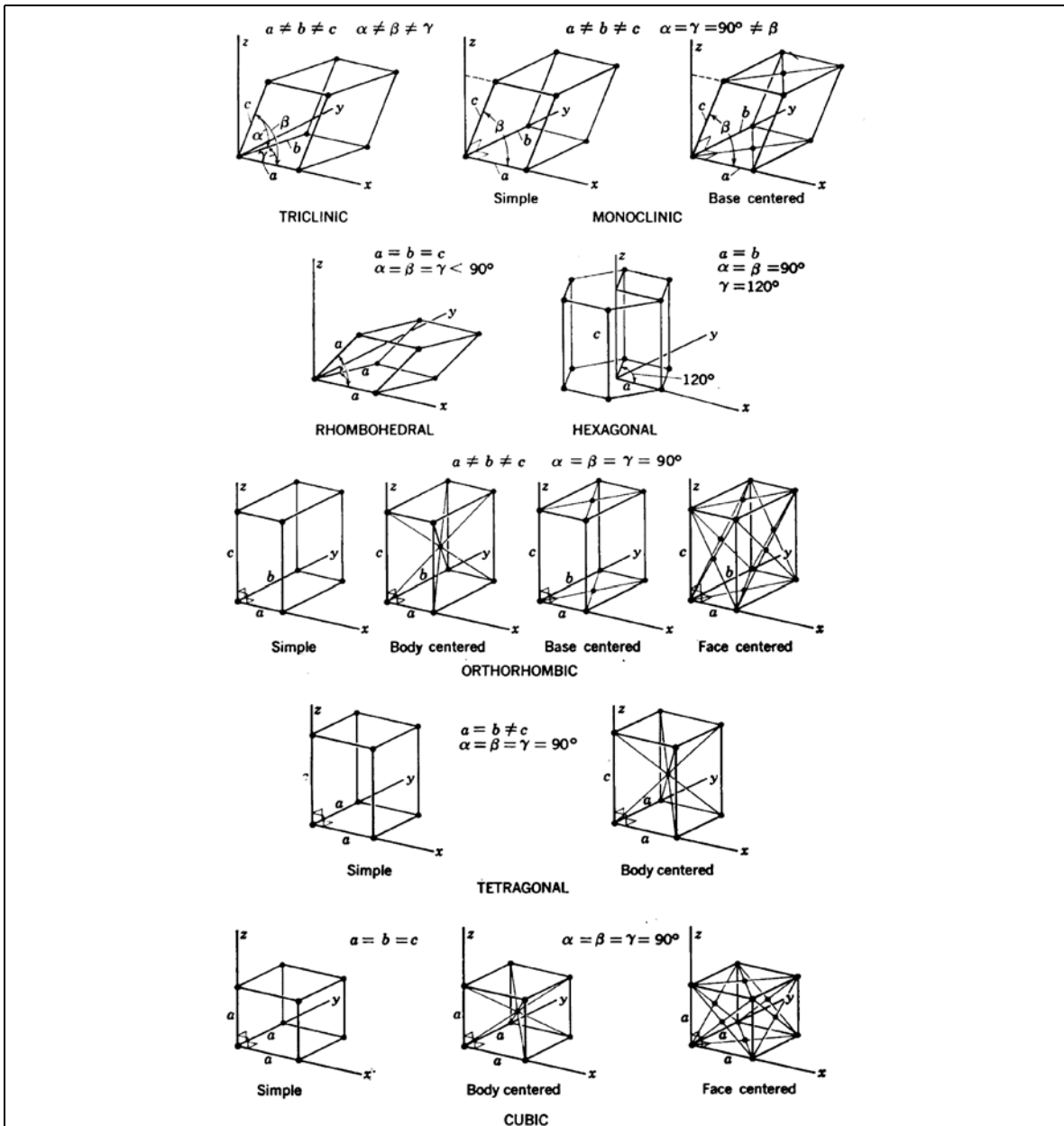


From geometry, the distance between adjacent planes is given by $d = \frac{s}{\sqrt{\alpha^2 + \beta^2 + \gamma^2}}$,
where s is the distance from one atom to its nearest neighbor in the cubic lattice.

PROCEDURE

Here the object is to generate a plot of meter intensity vs. grazing angle, for two different Bragg planes.

1. Straighten the goniometer arms such that Transmitter and Receiver face each other directly; they will be at 0 and 180 degrees, respectively.
2. Put the rotating table on the goniometer and rotate it such that the angle indicator reads 0 degrees. Note that you will be recording **grazing angles**, not angles of incidence or reflection. Luckily the grazing angle is simply the complement of the incident angle.
3. Place the "crystal" on the rotating table in the center of the goniometer, with the exposed steel balls facing **up**. Identify the 100 Bragg plane (see page 6) and orient the crystal (without rotating the table underneath) such that the plane is initially parallel to both goniometer arms. Do **NOT** try to align the sides of the tube with the edges of the rotating table, since neither is a perfect square – instead, visually align the exposed steel balls with the straightened goniometer arms.
4. Reconnect the transmitter AC adapter and turn the receiver on. Adjust the multiplier and fine-tuning knobs on the receiver so that you read 0.5 on the scale. Make sure nothing (arms, head, books, etc) is close to the apparatus while you are making the reading, to minimize reflections, which may cause interference and give false measurements. Enter data in the table in the hand-in sheet, starting off with 0 degrees and 0.5 as your first data pair.
5. Turn the rotating table (and hence the crystal) **two** degrees clockwise and the moveable goniometer arm **four** degrees clockwise. What you are doing here is maintaining the incident angle the same as the reflected angle, a condition necessary for Bragg diffraction. Note the reading on the meter and record. Repeat, each time rotating table two degrees (four degrees for moveable arm) to take new reading. You may have to change the multiplier setting (30X, 10X, 3X) to get the meter needle within mid-range. Remember that, just like a multimeter with selectable ranges, switching to the the range that gives you the most significant digits in your measurement will improve the precision of your data.
6. Plot your data and note the peaks in the graph. Each peak corresponds to a maxima in the $2d \sin \theta = m\lambda$ equation. Recall that higher order maxima have greater angles. From this data and labeled frequency on the transmitter calculate the experimental plane separation d_{exper} (averaging data from peak(s)) and compare with the theoretical plane separation $d_{\text{theory}} = \frac{s}{\sqrt{\alpha^2 + \beta^2 + \gamma^2}}$, where s is measured on crystal directly with a ruler.
7. Repeat the steps above for another Bragg plane (110).



The fourteen possible types of crystal lattices and the relationships between their Miller Indices. In this particular diagram $\alpha\beta\gamma$ denote the angles the sides of the lattice make with the coordinate axes xyz ; the Miller indices are denoted by abc . No matter how complex the structure of the atoms are, the underlying lattice which these atoms are grouped belong to one of these fourteen types. Examining the lattice diagram for Table Salt earlier in this write-up, we can easily see that NaCl has a face-centered cubic lattice. (from *Principles of Modern Physics*, R. Leighton, McGraw-Hill, 1959)

Probing Atomic Crystals: Bragg Diffraction (Hand-in Sheets 9-14)

Name _____ Date _____

Lab Partner(s) _____

Simple Reflection

Transmitter Angle	Receiver Angle	Plate Angle	Angle of Incidence	Angle of Reflection

Bragg Diffraction

100 Bragg plane		110 Bragg plane	
_ (degrees)	Intensity (mA)	_ (degrees)	Intensity (mA)
0		0	
2		2	
4		4	
6		6	
8		8	
10		10	
12		12	
14		14	
16		16	
18		18	
20		20	
22		22	
24		24	
26		26	
28		28	
30		30	
32		32	
34		34	
36		36	
38		38	
40		40	
42		42	
44		44	
46		46	
48		48	
50		50	

Calculations (show all work)

$$2d \sin \theta = m\lambda ; \theta = \text{angle between incident wave and Bragg plane}$$

$$d = \frac{s}{\sqrt{\alpha^2 + \beta^2 + \gamma^2}}$$

Distance between two steel balls on crystal (non-diagonal measurement with ruler):

Calculate the theoretical distance between 100 Bragg planes:

Calculate the experimental distance between 100 Bragg planes:

Calculate the theoretical distance between 110 Bragg planes:

Calculate the experimental distance between 110 Bragg planes:

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Questions

1. Describe what modifications the apparatus would need for you to observe the 111 plane.
2. How close (give a percentage) were your values for d_{exper} and d_{theory} ?
3. What possible sources of error are there in your measurements, and **please don't say "human error"**.
4. Suppose the "crystal" was shrouded, so that you couldn't see the exposed steel balls and you had no idea how they were arranged – how would you approach trying to guess their arrangement?

