X-Ray Diffraction Review Questions

Instructor's Guide

1. It is now possible to grow certain solids virtually an atomic layer at a time. Consider solid **A,** formed exclusively from copper and gold atoms, in which two atomic layers of gold atoms are put down, followed by two atomic layers of copper atoms, followed by two atomic layers of gold atoms, etc. The cycle is repeated until the desired thickness is reached, say, 100 atomic layers of each kind of atom; this is shown schematically below with X's and O's being Cu and Au, respectively.

   XXXXXXXXX
   XXXXXXXXX
   OOOOOOOOO   cross-sectional view of solid **A**
   OOOOOOOOO   **X = Cu; O = Au**
   XXXXXXXXX
   XXXXXXXXX
   OOOOOOOOO
   OOOOOOOOO etc.

   In preparing solid **B,** in contrast, the growth is changed after each layer: an atomic layer of Cu is grown, then an atomic layer of Au, then another atomic layer of Cu, etc:

   XXXXXXXXX
   OOOOOOOOO   cross-sectional view of solid **B**
   XXXXXXXXX   **X = Cu; O = Au**
   OOOOOOOOO etc.

   Why can diffraction be used to tell the two solids apart?

   The different structures create unit cells of different sizes, which, in turn, cause different diffraction patterns.

2. a. Infrared light and ultraviolet light can be used to generate a diffraction pattern from an array like those you worked with in lab. If your eyes were sensitive to infrared (IR) light with a wavelength of 8000Å and to ultraviolet (UV) light with a wavelength of 3000Å, using Fraunhofer's diffraction equation $\lambda = d \sin\varphi$ with d equal to the spacing between the lines in the diffraction grating (in this case 1.0×10^6Å), find the values for φ and compare them.

IR	UV
$\lambda = d \sin\phi$	$\lambda = d \sin\phi$
$8000 = 1.0 \times 10^6$Å$(\sin \phi)$	$3000 = 1.0 \times 10^6$Å$(\sin \phi)$
$\sin \phi = 8.0 \times 10^{-3}$	$\sin \phi = 3.0 \times 10^{-3}$
$\phi = 0.46°$	$\phi = 0.17°$

   The IR light, which has a longer wavelength, has a larger angle, and UV has a shorter wavelength and a smaller angle.

   b. What difference would you see in the diffraction patterns produced by these two types of light?

(Students may have a hard time answering this.)

The angle and therefore the size of the diffraction pattern increases with the wavelength of light used. You can see this, if you look back at *Appendix A* which shows Fraunhofer diffraction. Mathematically, students should understand that the side opposite the larger angle will be larger in size. Therefore, as shown in the diagram the side opposite the angle, ϕ, is calculated by d sinϕ. The distance between dots in a diffraction pattern is also calculated by d sinϕ. Therefore, UV radiation would lead to a small diffraction pattern, and IR radiation would yield a large diffraction pattern.

3. The diffraction equation for the slides you used in lab can be written as $d\,x = \lambda\,L$, where d is the spacing between dots on the slide; x is the spacing between spots in the resulting diffraction pattern; L is the distance from the slide to the screen (onto which the diffraction pattern is projected); and λ is the wavelength of light used. Using this equation, note which of the variables d, x, λ, and L are constant and which are changing as you answer the questions.

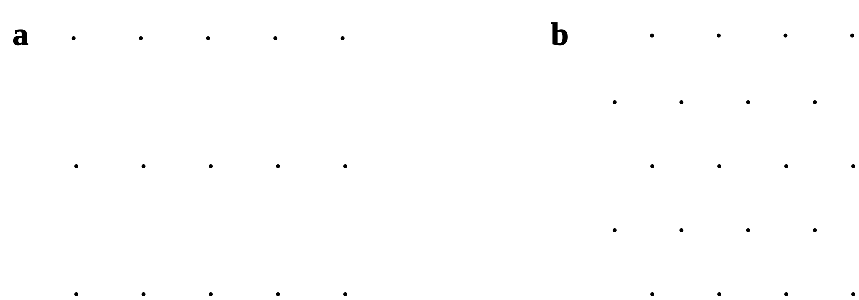
   a. If you have a given array with a laser light source, what happens to the size of the diffraction pattern if you move the slide farther from the screen?

      L is increasing. λ and d are held constant, so the equation predicts that x (the spacing between the diffraction spots) will increase. Therefore, the diffraction pattern should get larger as the length between the slide and the screen increases.

   b. If you use a given array with a white light source, what is the relative size of the diffraction pattern for red vs. violet light.

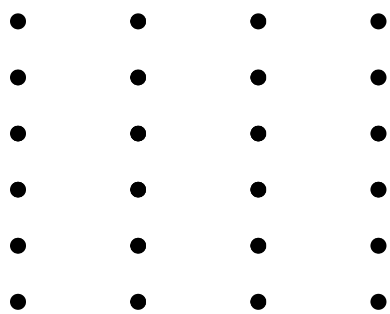
      For any array, the diffraction spots have a rainbow appearance with the red portion of the spots defining the largest diffraction pattern and the violet portion of the spots defining the smallest diffraction pattern. In terms of the equation, d and L are constants so that x = a constant times λ. The wavelength, λ, is larger for red light than for violet light, so x should be larger for red light than for violet light. Therefore, a larger diffraction pattern is expected for red compared to violet light.

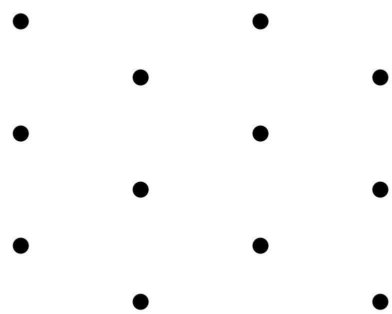
4. The two arrays of dots, **a** and **b**, are identical except that in array **b** there is an extra dot in the middle of each rectangle formed by four neighboring dots in array **a**.



Using the same experimental conditions (same wavelength and distance from the array to the screen where diffraction is observed), the diffraction patterns for the two arrays are found to be identical, except that every other diffraction spot is missing from one of the patterns, as shown below. Call the diffraction pattern on the left **X** and that on the right **Y**.

X **Y**





a. Based on your laboratory observations, which of the two diffraction patterns **X** and **Y** corresponds to array **a** and which to array **b**?

Diffraction pattern X corresponds to array a and diffraction pattern Y corresponds to array b: what was seen in lab with square arrays was that adding an extra dot to the middle of the array caused every other diffraction spot to disappear.

b. Explain why having additional dots in the centers of the array of rectangles (array **b** relative to array **a**) has the effect you describe in part *a* on the diffraction pattern.

The extra dots in the middle of the array cause destructive interference.

c. Compare the relative sizes of unit cells for arrays **a** and **b**. What happens to the relative sizes of their diffraction patterns?

Array a has a larger unit cell than array b (see Figure). However, the diffraction pattern of a would be smaller than that of b because there is an inverse relationship that exists between the spacing between the dots in the array and spots projected in the diffraction pattern (reciprocal lattice effect).

5. It has been predicted that if we could put the element hydrogen, normally an invisible gas of diatomic molecules at room temperature and pressure, under sufficiently high pressure – millions of atmospheres - it would become a metal!

   If you could conduct a diffraction experiment on the hydrogen sample while it was being squeezed, what do you predict would happen to the spacing between diffraction spots as the atoms are placed under increasing pressure and why?

   An increase in pressure should cause the atoms to become closer together, and the spacing between spots of the diffraction pattern would consequently increase: Recall that dx = constant, i.e., atomic spacing and their diffraction spot spacing are inversely related.

6. As mentioned in class, relative atomic positions in crystals are generally determined by diffraction experiments. The optical transform slide was used to investigate diffraction effects: the photographically-reduced dot arrays on your slide represent arrays of atoms in a crystal. The diffraction equation for the slide you used can be written as $dx/L = \lambda$, where d is

the distance between the dots on the slide; x is the distance between the spots of the resulting diffraction pattern; L is the distance between the slide and the surface where the diffraction pattern is observed; and λ is the wavelength of light used for the experiment. For your experiment, you can observe a distant point source of white light through your slide (a street lamp, e.g.); and/or a point source of colored light, like your LED from lab or a traffic light.

a. Design and interpret an experiment using the Discovery slide to show that *d* and *x* are inversely related.

In array "b" there is a smaller spacing (value of d) than in array "d." If we keep the viewing arrangement of a light source constant (L and λ constant), then dx = constant, predicting that the size of the diffraction pattern, x, and the dot spacing on the slide, d, are inversely related. You should see that array "d" gives a smaller diffraction pattern than array "b."

b. Design and interpret an experiment to show that x and λ are directly related.

If you look at any single array from a fixed distance, you are keeping d and L constant, so that x/λ = constant, meaning they are directly related. You should see by looking at a white light source, e.g., that the longer wavelength red light gives a larger diffraction pattern (value of x), than shorter wavelengths of light that occur toward the violet part of the spectrum.

7. A sample of Fe, like many materials, expands as it is warmed. What will happen to the size of the diffraction pattern as the sample is warmed why?

There is an inverse relationship between atom spacing and diffraction spot spacing, if the wavelength and spot-to-screen separation remain constant during an experiment. Thus, the diffraction pattern should contract as the material expands with heating.