X-Ray Diffraction Review Questions

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.

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XXXXXXXXXX
XXXXXXX
OOOOOOOOOO  cross-sectional view of solid A
OOOOOOOOOO  X = Cu; O = Au
XXXXXXX
XXXXXXX
OOOOOOOOOO
OOOOOOOOOO 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:

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XXXXXXXXXX
OOOOOOOOOO  cross-sectional view of solid B
XXXXXXX     X = Cu; O = Au
OOOOOOOOOO etc.
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Why can diffraction be used to tell the two solids apart?

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 $\lambda = d \sin \phi$ with $d$ equal to the spacing between the lines in the diffraction grating (in this case $1.0 \times 10^6$Å), find the values for $\phi$ and compare them.
b. What difference would you see in the diffraction patterns produced by these two types of light?

3. The diffraction equation for the slides you used in lab can be written as \( d \times x = \lambda \times L \), 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 \( \lambda \) is the wavelength of light used. Using this equation, note which of the variables \( d \), \( x \), \( \lambda \), 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?

   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.

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 \( a \).

\[
\begin{array}{cccc}
\text{a} & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\end{array}
\begin{array}{cccc}
\text{b} & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
\end{array}
\]

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

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.

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

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?
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 $\lambda$ 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.

   b. Design and interpret an experiment to show that $x$ and $\lambda$ are directly related.

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?