

# X –ray diffraction

## Preparatory questions

1. What are X-Rays? Why do we use x-rays to examine crystal structures? How are the x-rays in this experiment produced?
2. What is Bragg's law? How does it explain the lines obtained in the X-ray diffraction powder method?
3. For a cubic crystal Bragg's law can be rewritten as  $\sin^2 \theta = \left( \frac{\lambda^2}{4a^2} \right) (h^2 + k^2 + l^2)$ ,  
 where  $(h,k,l)$  are the Miller indices characterizing the set of diffracting planes. Briefly describe the connection between the Miller indices and diffraction planes.
4. Complete the table of the Miller indices associated with X-ray diffraction lines for the three crystals: Simple cubic, body centered cubic (BCC), and face centered cubic (FCC)

| Simple Cubic<br><i>(h k l)</i> | Body Centered<br>Cubic <i>(h k l)</i> | Face Centered<br>Cubic <i>(h k l)</i> | $h^2 + k^2 + l^2$ |
|--------------------------------|---------------------------------------|---------------------------------------|-------------------|
|                                |                                       |                                       | 1                 |
|                                |                                       |                                       | 2                 |
|                                |                                       |                                       | 3                 |
|                                |                                       |                                       | 4                 |
|                                |                                       |                                       | 5                 |
|                                |                                       |                                       | 6                 |
|                                |                                       |                                       | 8                 |
|                                |                                       |                                       | 9                 |
|                                |                                       |                                       | 10                |
|                                |                                       |                                       | 11                |
|                                |                                       |                                       | 12                |

5. Which type of X-rays—Bremsstrahlung or K-shell emission—is best for measuring X-ray diffraction and why?
6. 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?