

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. Which type of X-rays—Bremsstrahlung or K-shell emission—is best for measuring X-ray diffraction and why?
3. What is Bragg's law? How does it explain the lines obtained in the X-ray diffraction powder method?
4. 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.
5. Complete the table of the Miller indices associated with X-ray diffraction lines for the following crystals: Simple cubic, body centered cubic (BCC), face centered cubic (FCC) and (FCC –diamond). For any given value of $s=h^2 + k^2 + l^2$, list all allowed values of (h,k,l) . Note that the structure of Si is identical to that of diamond.

Simple cubic (hkl)	BCC (hkl)	FCC (hkl)	FCC-diamond (hkl)	$s=h^2 + k^2 + l^2$
				1
				2
				3
				4
				5
				6
				8
				9
				10
				11
				12

6. Explain the reason for “missing lines” in X-ray spectra. In other words why for certain crystal structures there are values of hkl that do not produce a peak in an X-ray 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?