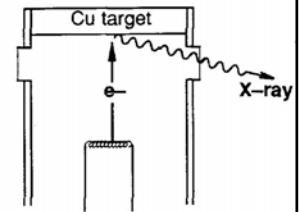


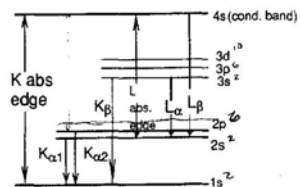
X-ray Diffraction

X-ray Generation

- X-ray tube (sealed)
- Pure metal target (Cu)
- Electrons remove inner-shell electrons from target.
- Other electrons “fall” into hole.

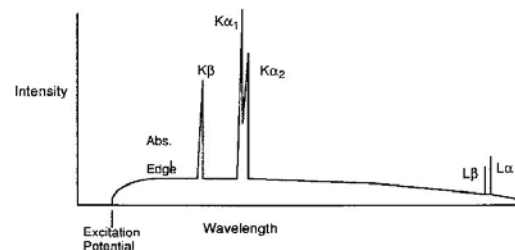


X-ray Generation



- The incoming electron must have enough energy to remove inner 1s electrons from the copper atoms.
- This energy corresponds to the Cu absorption edge
- The 2s and 2p electrons fall back into the 1s shell and emit the $K\alpha_1$ $K\alpha_2$ lines.

X-ray Spectrum from Tube



Energy Calculations

- Planck's constant (h) = 6.6×10^{-34} joule-sec
- 1 electron-volt = 1.6016×10^{-19} joule
- Speed of light (c) = 3.0×10^8 m/s
- Photon frequency $\nu = c/\lambda$
- Photon Energy $E = h\nu = hc/\lambda$

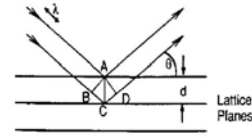
Energy Calculations

- What is the minimum potential in KV that is required to excite Cu K-series radiation from a Cu-target X-ray tube?
- Absorption edge of Cu = 1.380\AA
- $E = hc/\lambda = (6.60 \times 10^{-34})(3 \times 10^8)/(1.380 \times 10^{-10})$
- $E = 1.435 \times 10^{-15}$ joule
- $E = 1.435 \times 10^{-15} / 1.6016 \times 10^{-19} = 8958$ ev
- The potential on the tube must exceed 8.958 KV

Diffraction

- Diffraction is the coherent scattering of waves from a periodic array of scatterers.
- The wavelength of light is about half a micron
- Light is diffracted by the tracks in a CD.
- The wavelengths of X-rays is about the same as the interatomic distances in crystals.

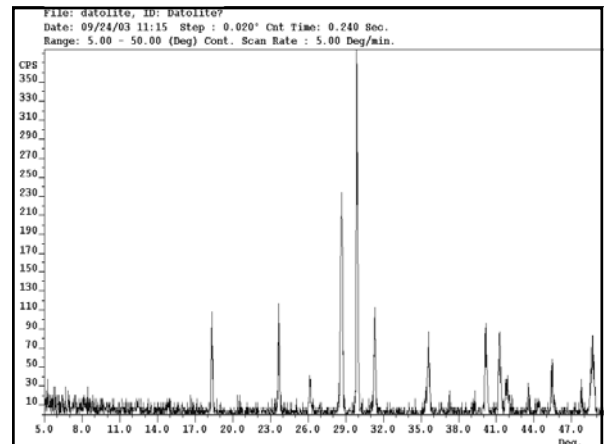
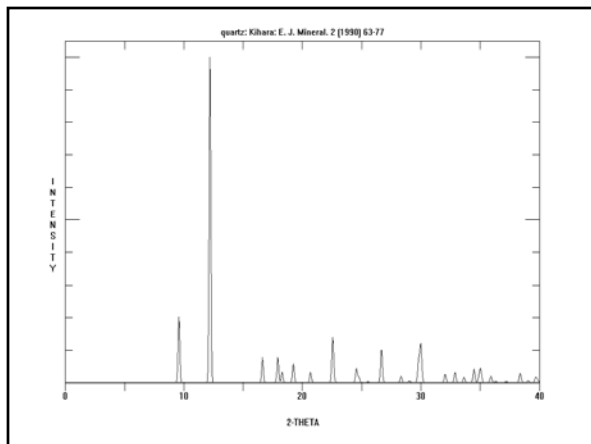
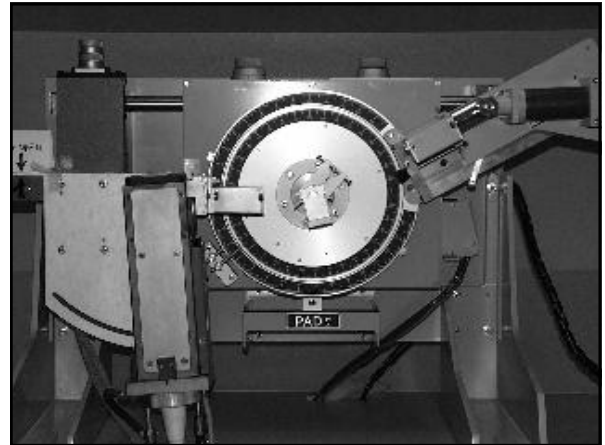
X-Ray Diffraction

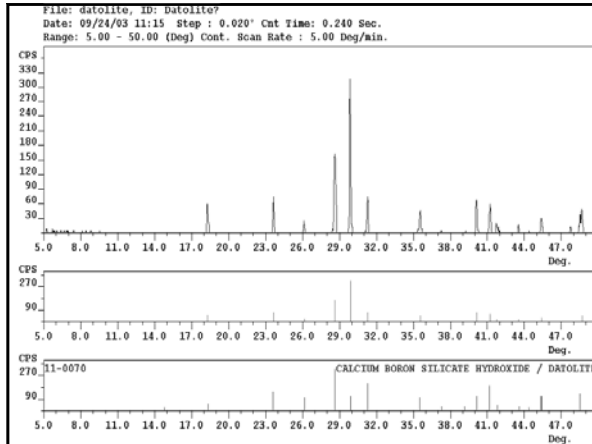


- Atoms separated by distance d will scatter in phase when the path length difference is an integral number of wavelengths.
- Path length difference $B-C-D = n\lambda$
- $n\lambda = 2d \sin \theta$

X-ray Diffraction Experiment

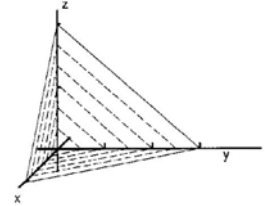
- We use the 'monochromatic' $K\alpha_{1-2}$ lines for our diffraction experiment.
- The wavelength is 1.5405\AA
- We use a diffracted beam monochromator to clean up the X-rays entering the detector.
- We use a powdered sample so that all orientations are present in the sample.
- We move the detector through angle 2θ .





Miller Indices

- The real use of Miller indices is to describe diffraction planes.
- For a lattice plane with Miller indices $h k l$ in an orthorhombic lattice $a b c$,
- $d = 1 / [(h/a)^2 + (k/b)^2 + (l/c)^2]^{1/2}$
- For cubic:
- $d = a/[h^2 + k^2 + l^2]^{1/2}$



Diffraction Calculations

- For forsterite $a = 4.75$; $b = 10.20$; $c = 5.98\text{\AA}$
- Calculate 2θ for the (201) lattice spacing for $\text{CuK}\alpha$ ($\lambda = 1.5405\text{\AA}$)
- $d = 1 / [(h/a)^2 + (k/b)^2 + (l/c)^2]^{1/2}$
- $d = 1 / [(2/4.75)^2 + (1/10.20)^2 + (1/5.98)^2]^{1/2}$
- $d = 1/0.4530 = 2.207\text{\AA}$
- $2\theta = 2 \sin^{-1} \lambda/2d = 2 * \sin^{-1} (1.5405/4.414)$
- $2\theta = 2 * 20.43 = 40.86^\circ$

XPOW

- XPOW uses the unit cell and atom position data to calculate the diffraction pattern.
- Intensities can be calculated knowing the position and scattering characteristics of each atom.
- F_{hkl} = square root of integrated intensity.
- f_j = scattering of atom j at angle 2θ
- Atom j located at fractional coordinates x_j, y_j, z_j .

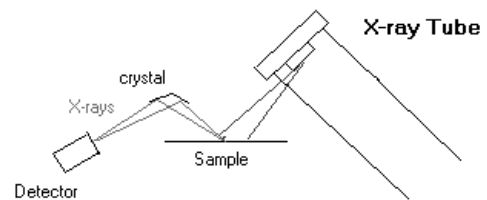
$$F_{hkl} = \sum_{j=1}^n f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

Uses of X-ray Powder Diffraction

- Mineral identification
- Determination of Unit Cell Parameters
- Modal (phase percentage) Analysis
- Crystal Structure Determination

X-ray Fluorescence

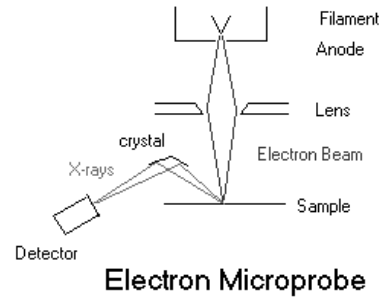
X-ray Fluorescence



X-ray Fluorescence

- *Chemical analysis*
- *Major and minor element*
- *Uses Ag $k\alpha$ to excite secondary X-rays from sample.*
- *Powdered or flux-fused glass sample.*

Electron Microprobe



Electron Microprobe

- *Chemical analysis*
- *Major and minor element*
- *Uses electrons to excite secondary X-rays from sample.*
- *Electrons can be focussed onto a $10\mu\text{m}$ spot*
- *Sample is polished thin section*