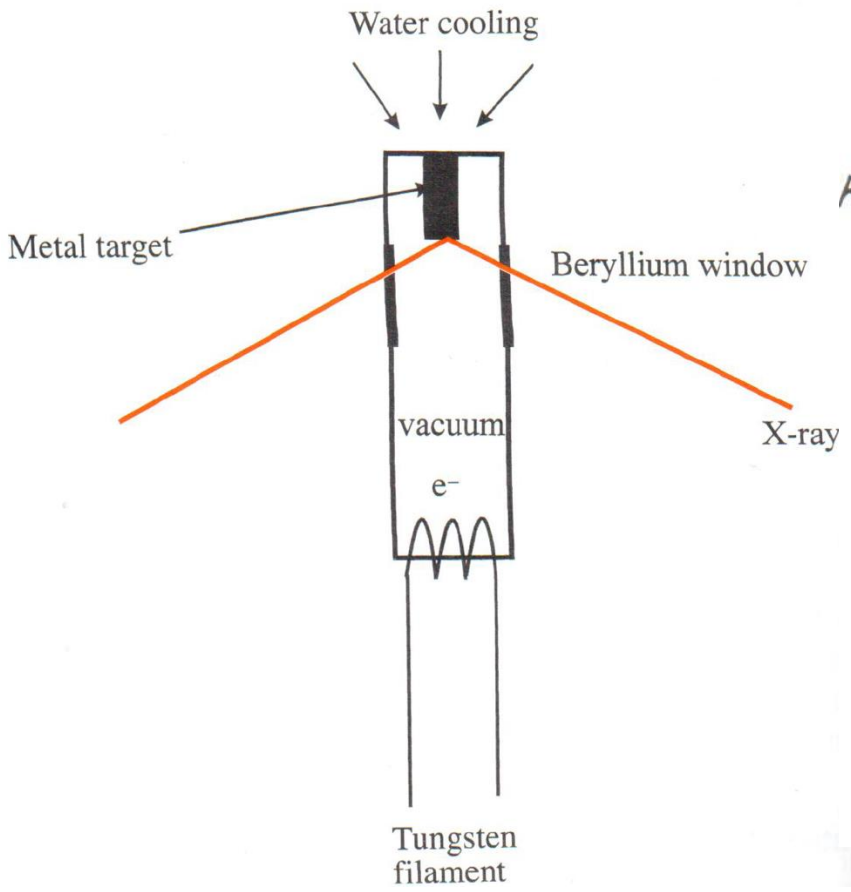
Module 2
Synthesis and Characterization

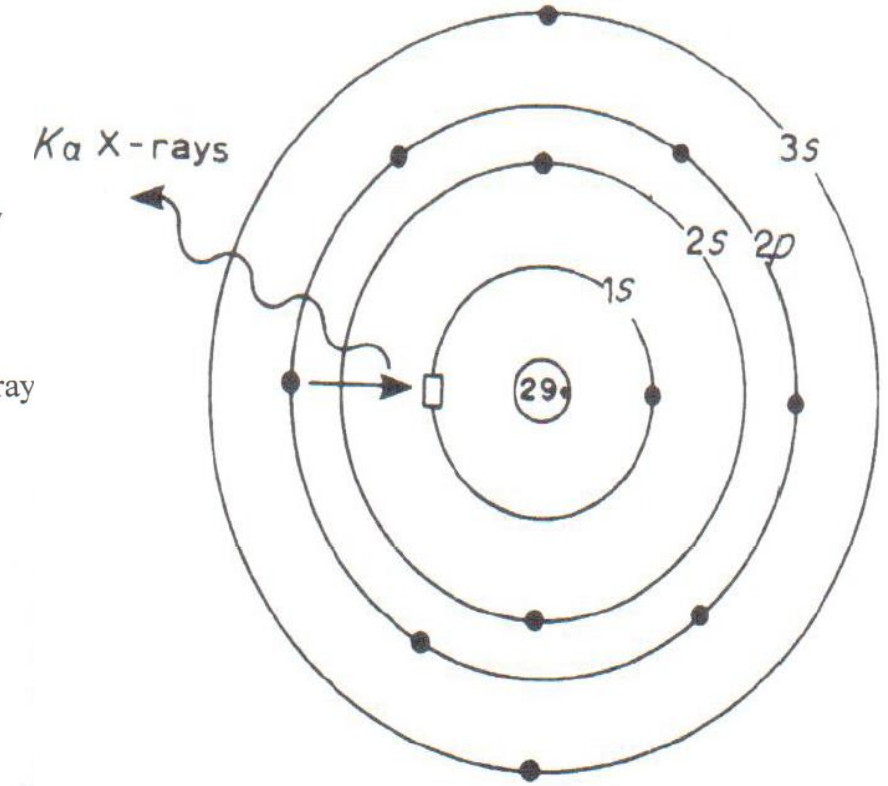
Solid State Chemistry and Energy

X-ray Generation

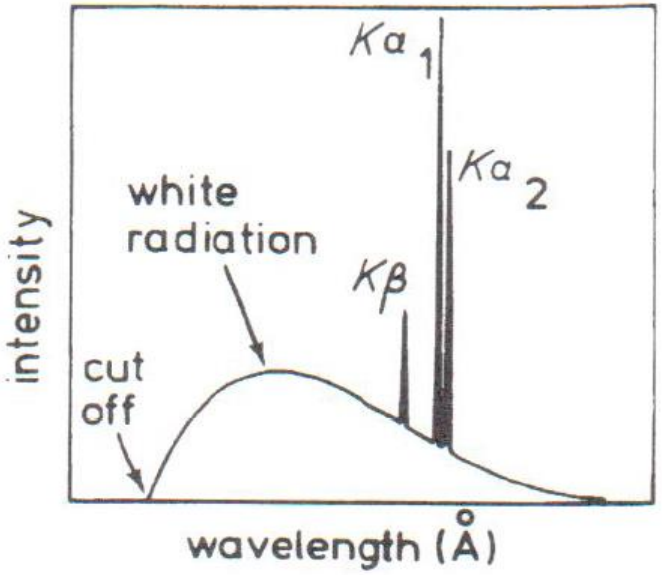
X-ray tube



X-ray emission



X-ray emission spectrum



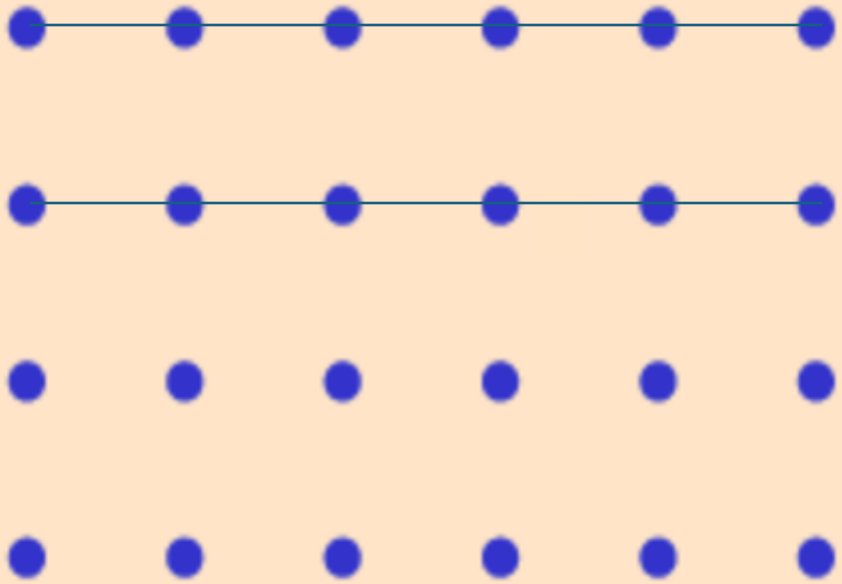
Common Sources

Table 3.2 *X-ray wavelengths (Å) of commonly used target materials*

Target	$K\alpha_1$	$K\alpha_2$	$K\bar{\alpha}^*$	Filter
Cr	2.2896	2.2935	2.2909	V
Fe	1.9360	1.9399	1.9373	Mn
Cu	1.5405	1.5443	1.5418	Ni
Mo	0.7093	0.7135	0.7107	Nb
Ag	0.5594	0.5638	0.5608	Pd

* $\bar{\alpha}$ is the intensity-weighted average of α_1 and α_2.

Bragg's Law



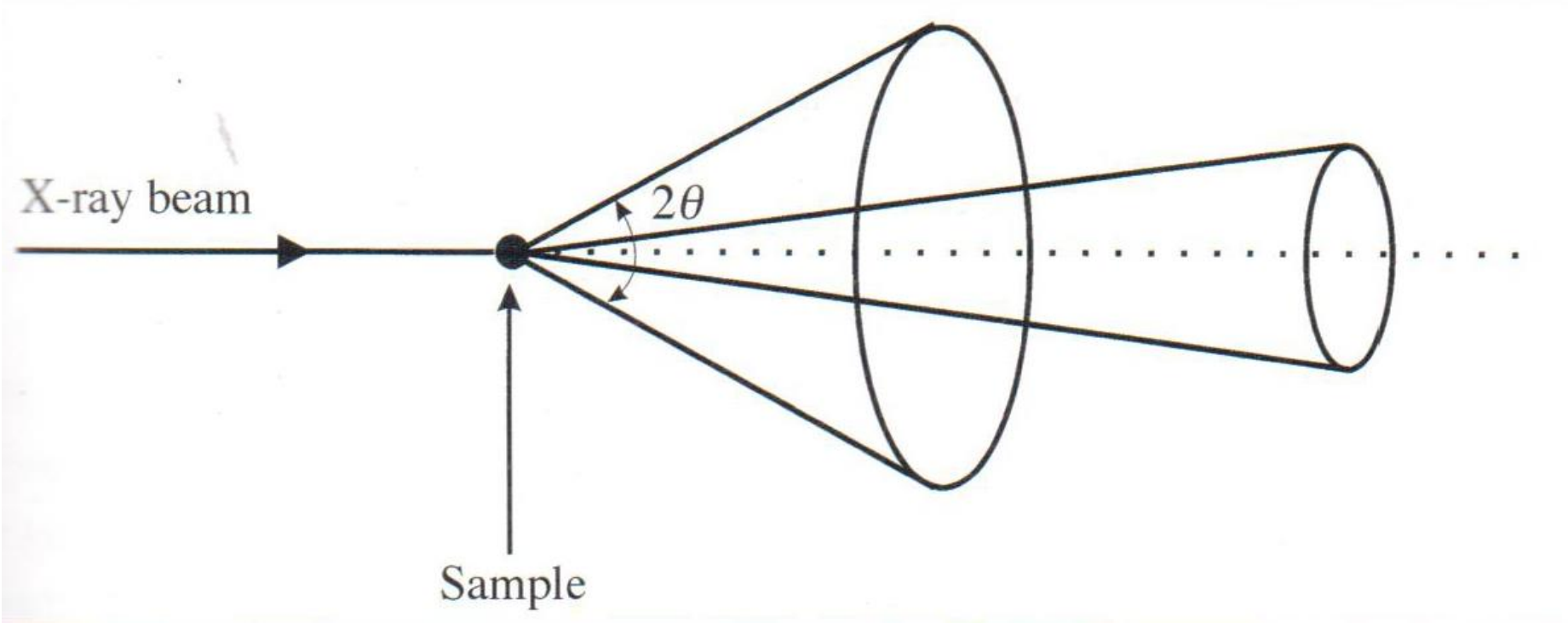
Two parallel planes of atoms

$\sin\theta$ = opp/hyp
hypotenuse = d-spacing
$d\sin\theta$ = opp

to an integer of the
structive interference!

Bragg's Law:
$n\lambda = 2d\sin\theta$

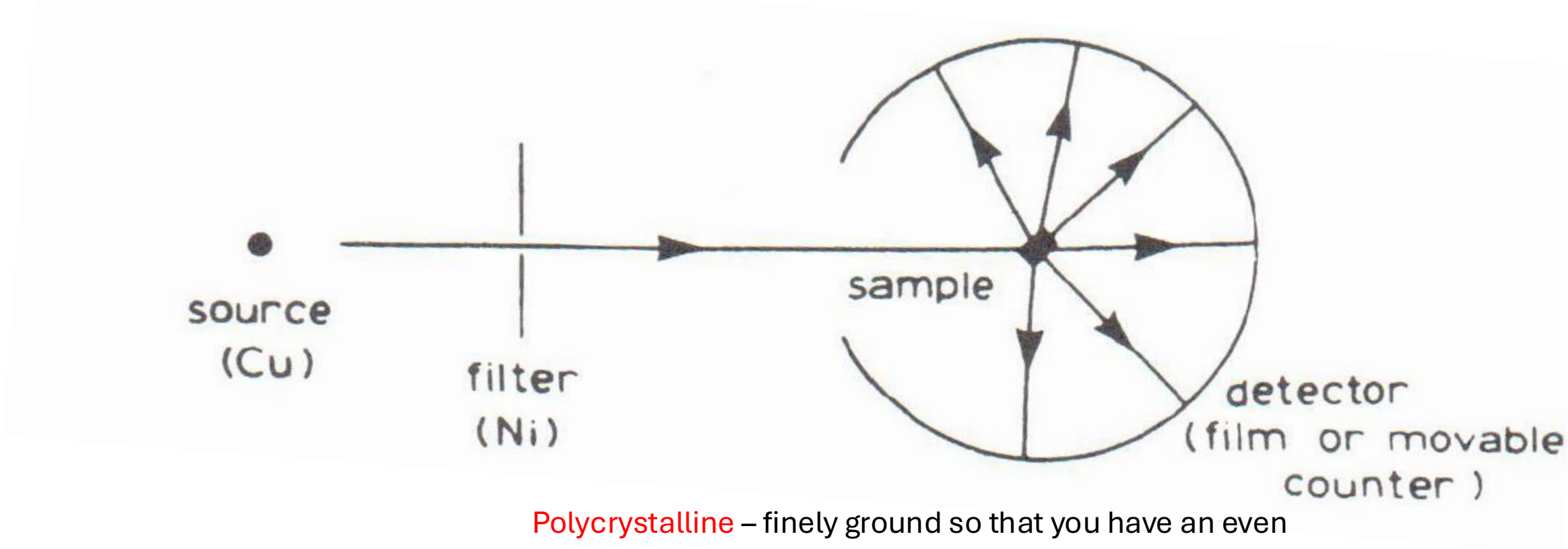
Powder x-ray diffraction experiment



Polycrystalline – finely ground so that you have an even distribution of orientations of your crystallites.

Exercise: What if the crystallites have column morphology? How do you expect the morphology to influence the resulting powder pattern?

Powder x-ray diffraction experiment



Polycrystalline – finely ground so that you have an even distribution of orientations of your crystallites.

Exercise: What if the crystallites have column morphology? How do you expect the morphology to influence the resulting powder pattern?

Exercise: Using Bragg's law calculate the 2theta value for a d-spacing of 20 Å and also for 1 Å both Cu and Mo radiation with wavelengths of 1.54 Å and 0.71Å, respectively.

Answer:

$n\lambda = 2d\sin(\theta)$

For Cu:

$1.54 = 2d\sin(\theta)$

$1.54/(2*20) = \sin(\theta)$, $\theta = 2.2$ so 2θ is $4.4°$

$1.54/(2*1) = \sin(\theta)$, $\theta = 50.35$ so 2θ is $100.71°$

For Mo:

$0.71 = 2d\sin(\theta)$

$0.71/(2*20) = \sin(\theta)$, $\theta = 1.01$ so 2θ is $2.03°$

$0.71/(2*1) = \sin(\theta)$, $\theta = 20.79$ so 2θ is 40.58