CHOICE OF X-RAY SOURCES

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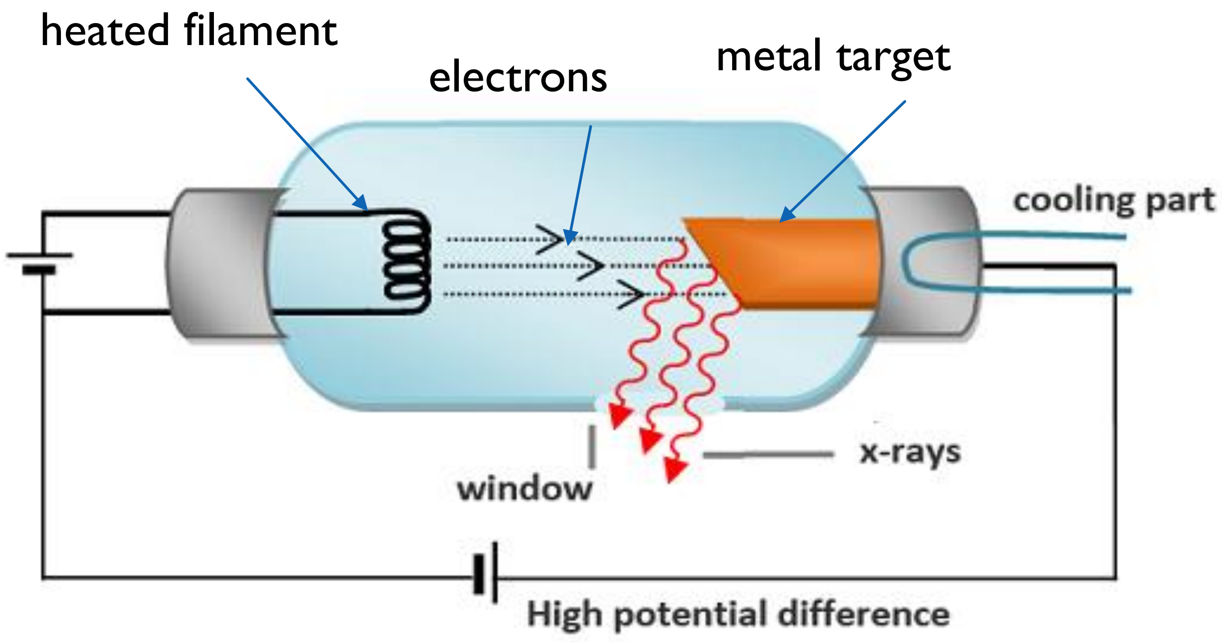
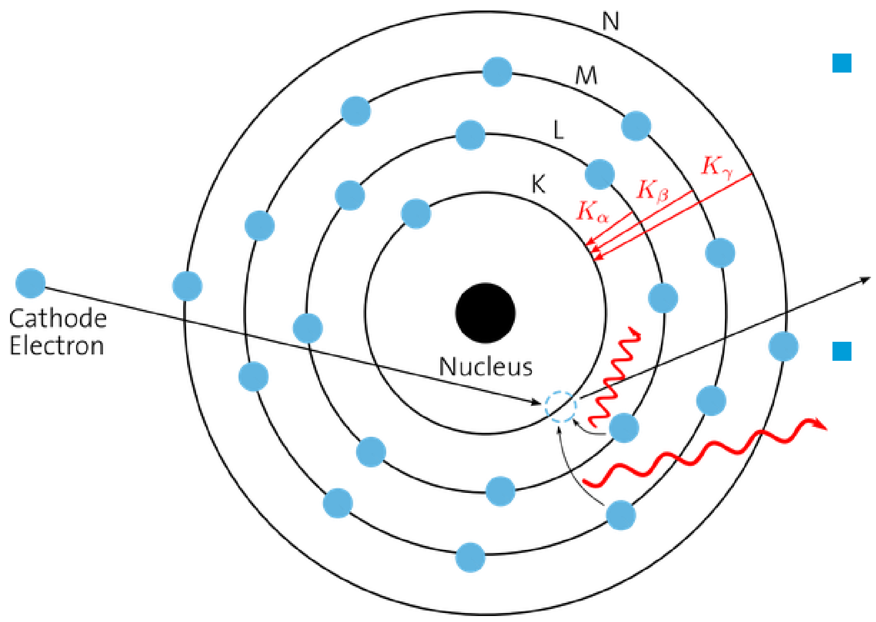
GENERATION OF X-RAYS



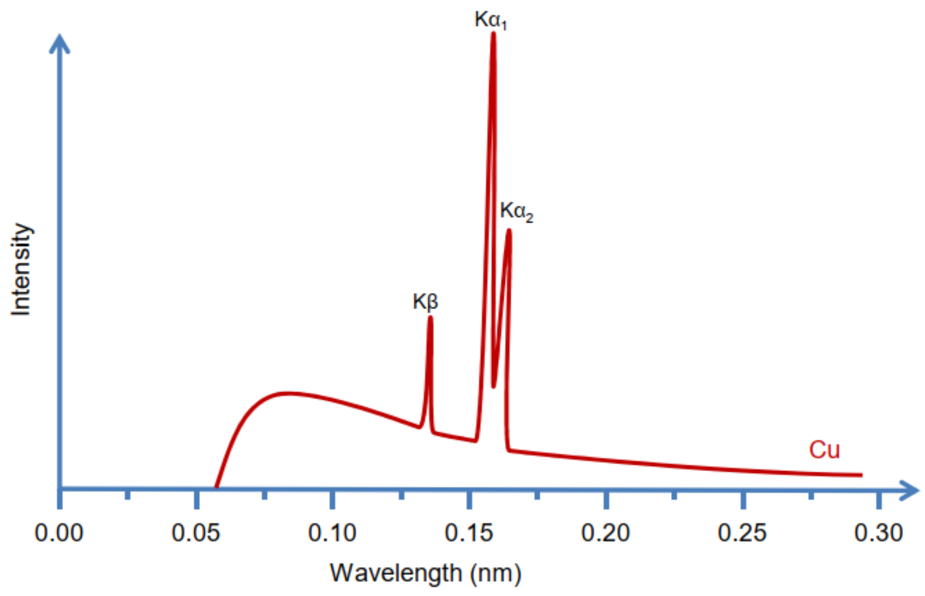
- X-rays are generated when matter is irradiated by a beam of high-energy charged particles such as electrons.
- In the lab, a filament is heated to produce electrons, which are accelerated in vacuum by a high electric field in the range of 20-60kV towards a metal target (namely anode).
- Nearly 99% of the beam energy will be dissipated as heat and only 1% of will produce the X-ray pattern.

CHARACTERISTIC RADIATION



- In a copper X-ray spectrum, it produces 3 characteristic lines, $K_{\alpha 1}$, $K_{\alpha 2}$, and K_{β}.

- In general, K_{α} is observed as a doublet peak in the XRD pattern and K_{β} is fileted out by a metal foil during the measurement.



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Wavelengths of typical X-ray anode materials

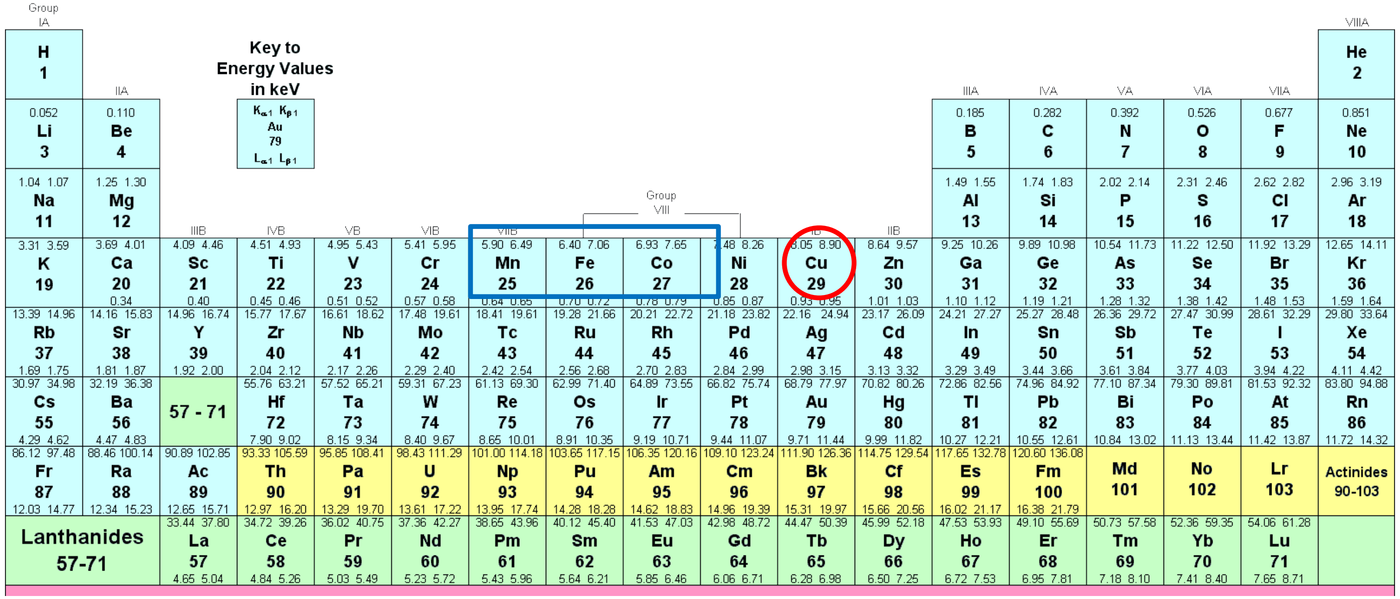
Anode materials	K_{α} (Average)	$K_{\alpha 1}$	$K_{\alpha 2}$	K_{β}
Cr	2.291	2.2897	2.29361	2.08487
Fe	1.93736	1.93604	1.93998	1.75661
Co	1.79026	1.78897	1.79285	1.62079
Cu	1.54184	1.54056	1.54439	1.39222
Mo	0.71073	0.7093	0.71359	0.63229
Ag	0.56088	0.55942	0.56381	0.49708

- Copper anode is by far the most common source, as its wavelength (1.54 Å) matches the interatomic distance of crystalline solid materials.
- Mo is commonly used for characterising single crystals and Cr source is used for stress measurement and materials with large unit cells.
- Cobalt source is used for samples rich in Fe, Co and Mn, to eliminate fluorescence effect.

Requirements of Anode Materials

- Be metals to conduct electrons
- reasonably high melting point (45kV and 40mA generates 1.8kW heat)

WHEN SHALL WE CHOOSE A COBALT ANODE?

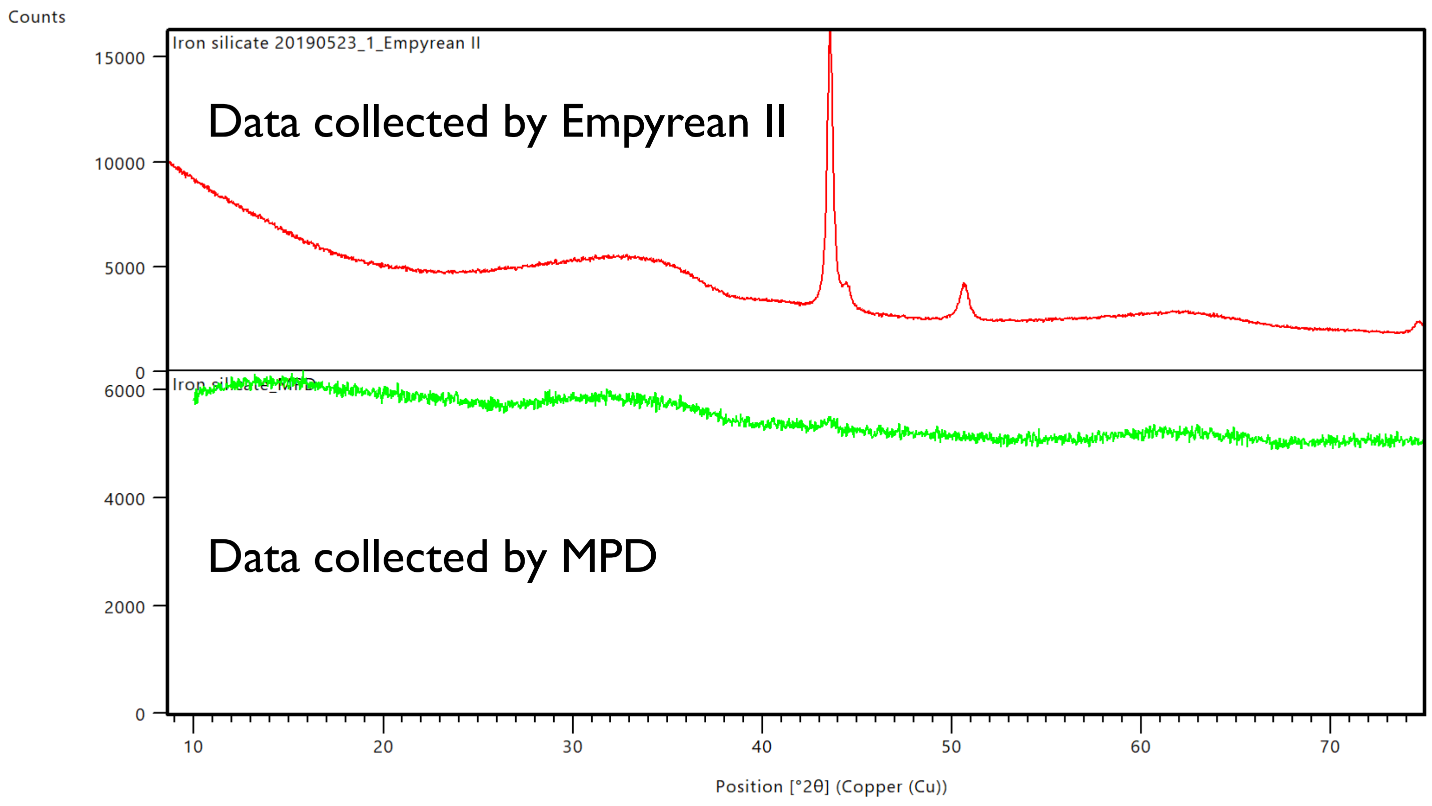


	$K_{\alpha I}$ emission energy (keV)	K-edge absorption energy (keV)
Cu	8.05	
Co		7.71
Fe		7.11
Mn		6.54

- For sample rich in Fe, Co or Mn, it will absorb a large amount of X-ray beam generated from Cu anode, as their absorption energies are close to Cu emission energy
- The florescence effect produces a relatively high background to signal ratio

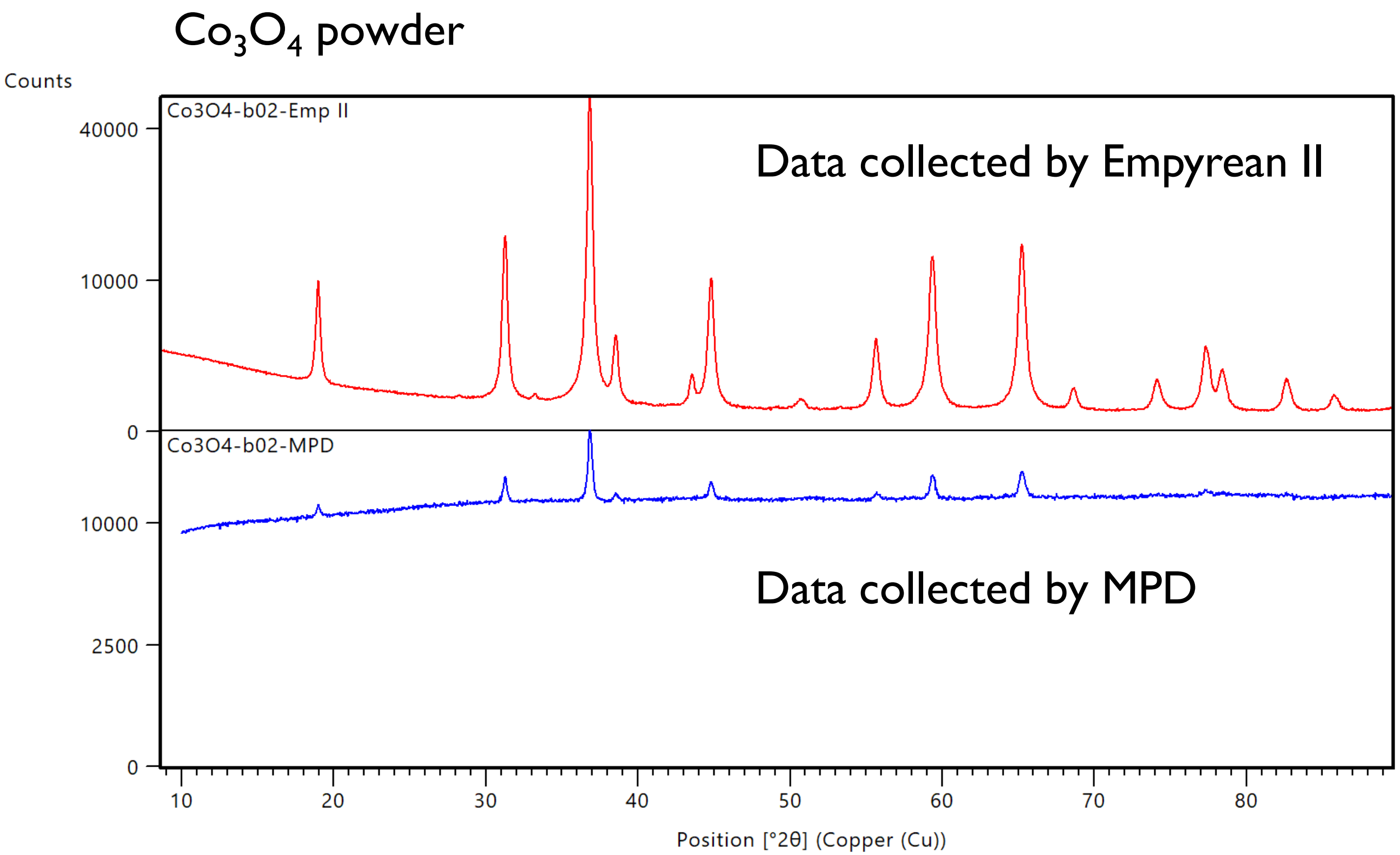
CASE STUDY 1

$FeSi_2$ powder



XRD raw data is provided by Yuting Yuan

CASE STUDY 2



XRD raw data is provided by Dr Yuan Wang

How to convert x-ray wavelengths by using Highscore Plus software?