



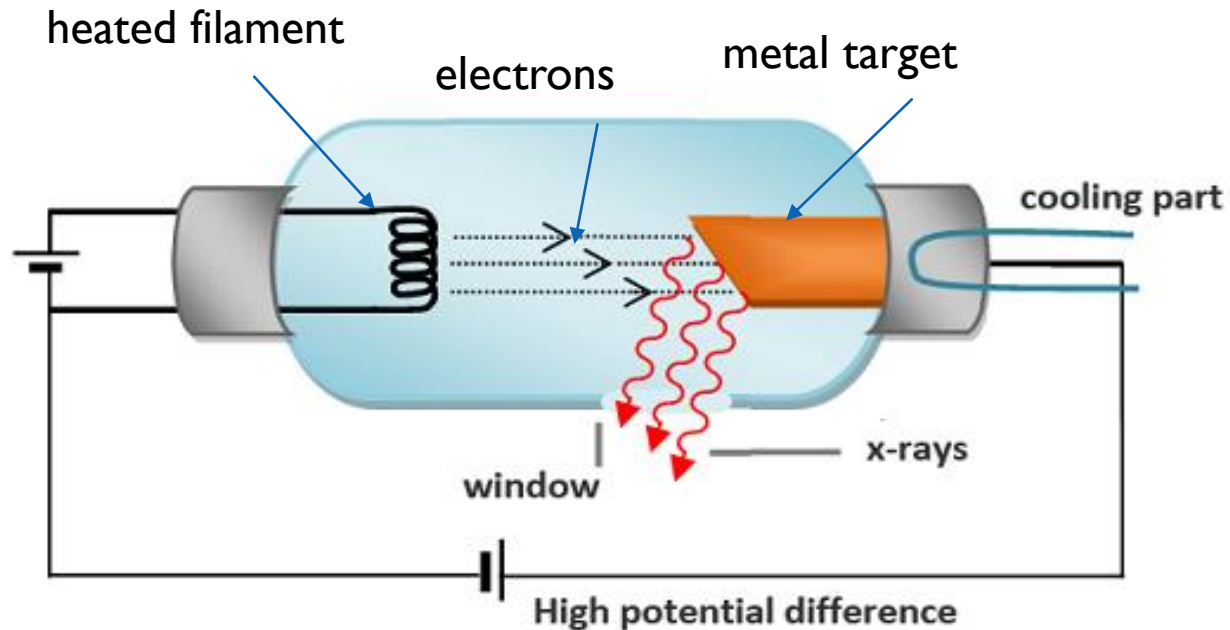
# CHOICE OF X-RAY SOURCES

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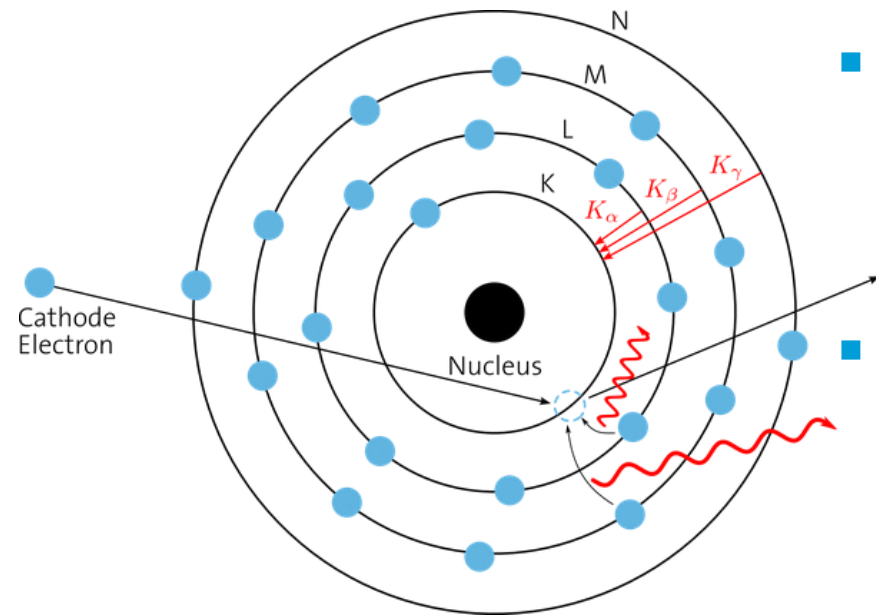
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# GENERATION OF X-RAYS

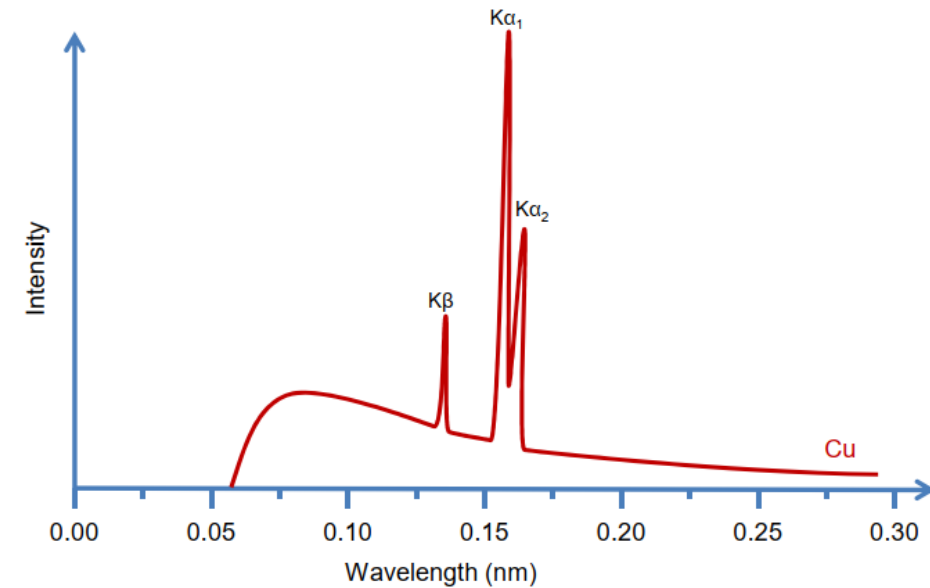


- X-rays are generated when matter is irradiated by a beam of high-energy charged particles such as electrons.
- In the lab, a filament is heated to produce electrons, which are accelerated in vacuum by a high electric field in the range of 20-60kV towards a metal target (namely anode).
- Nearly 99% 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  $K_\beta$ .
- In general,  $K_\alpha$  is observed as a doublet peak in the XRD pattern and  $K_\beta$  is filtered out by a metal foil during the measurement.



# CHOICE OF X-RAY SOURCES

Wavelengths of typical X-ray anode materials

Anode materials	$K_{\alpha}$ (Average)	$K_{\alpha 1}$	$K_{\alpha 2}$	$K_{\beta}$
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

## Requirements of Anode Materials

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

- **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.

# WHEN SHALL WE CHOOSE A COBALT ANODE?

Group IA

Key to Energy Values in keV  
 $K_{\alpha 1}$   
 $Au$  79  
 $L_{\alpha 1}$   $L_{\beta 1}$

Group VIII

VIIIA

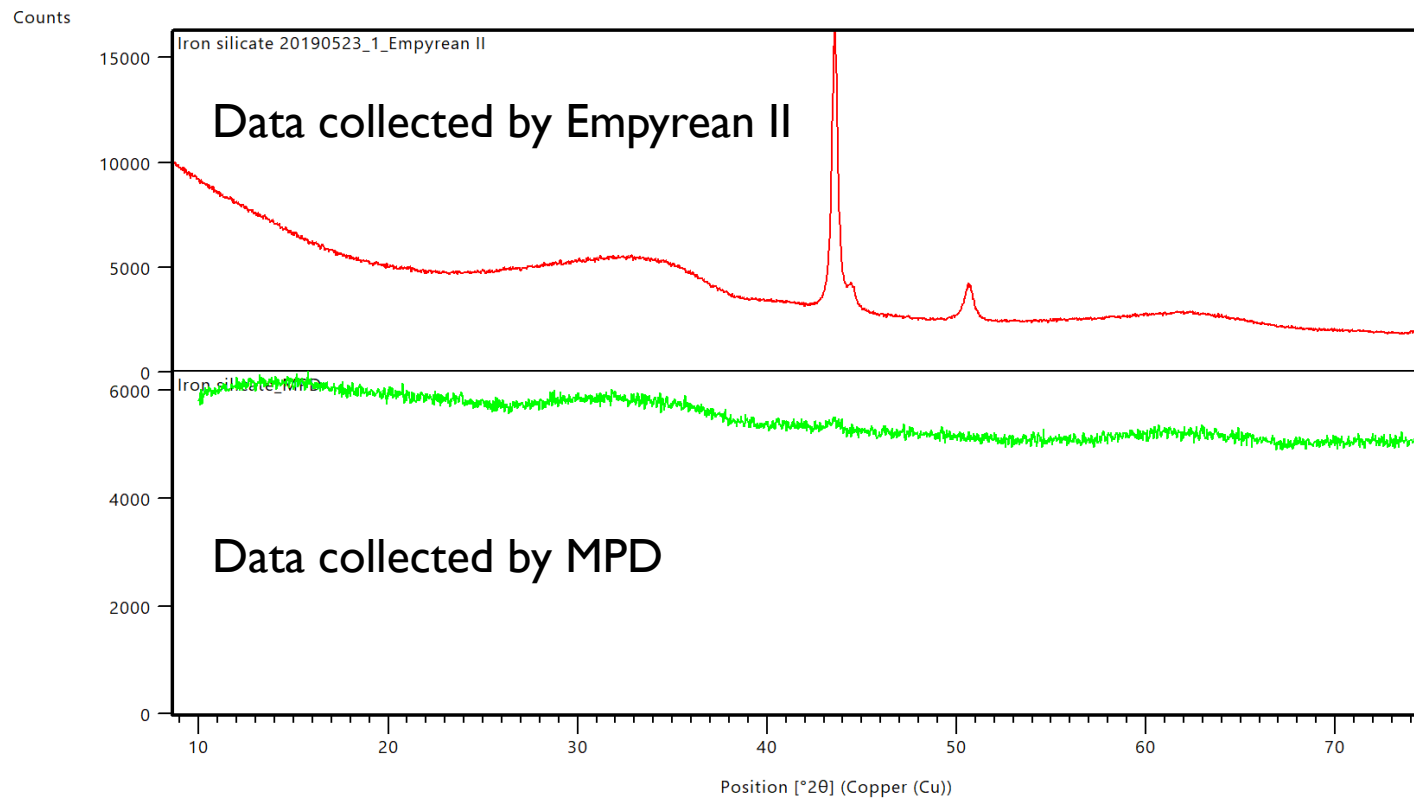
H 1																	He 2						
0.052 Li 3	0.110 Be 4																	0.185 B 5	0.282 C 6	0.392 N 7	0.526 O 8	0.677 F 9	0.851 Ne 10
1.04 1.07 Na 11	1.25 1.30 Mg 12																	1.49 1.55 Al 13	1.74 1.83 Si 14	2.02 2.14 P 15	2.31 2.46 S 16	2.62 2.82 Cl 17	2.96 3.19 Ar 18
3.31 3.59 K 19	3.69 4.01 Ca 20	4.09 4.46 Sc 21	4.51 4.93 Ti 22	4.95 5.43 V 23	5.41 5.95 Cr 24	5.90 6.49 Mn 25	6.40 7.06 Fe 26	6.93 7.65 Co 27	7.48 8.26 Ni 28	8.05 8.90 Cu 29	8.64 9.57 Zn 30	9.25 10.26 Ga 31	9.89 10.98 Ge 32	10.54 11.73 As 33	11.22 12.50 Se 34	11.92 13.29 Br 35	12.65 14.11 Kr 36						
13.39 14.96 Rb 37	14.16 15.83 Sr 38	14.96 16.74 Y 39	15.77 17.67 Zr 40	16.61 18.62 Nb 41	17.48 19.61 Mo 42	18.41 19.61 Tc 43	19.28 21.66 Ru 44	20.21 22.72 Rh 45	21.18 23.62 Pd 46	22.16 24.94 Ag 47	23.17 26.09 Cd 48	24.21 27.27 In 49	25.27 28.48 Sn 50	26.36 29.72 Sb 51	27.47 30.99 Te 52	28.61 32.29 I 53	29.80 33.64 Xe 54						
1.69 1.75 Cs 55	1.81 1.87 Ba 56	1.92 2.00 57 - 71	2.04 2.12 Hf 72	2.17 2.26 Ta 73	2.29 2.40 W 74	2.42 2.54 Re 75	2.56 2.68 Os 76	2.70 2.83 Ir 77	2.84 2.99 Pt 78	2.98 3.15 Au 79	3.13 3.32 Hg 80	3.29 3.49 Tl 81	3.44 3.66 Pb 82	3.61 3.84 Bi 83	3.77 4.03 Po 84	3.94 4.22 At 85	4.11 4.42 Rn 86						
30.97 34.98 Fr 87	32.19 36.98 Ra 88	33.44 37.80 Ac 89	34.72 39.26 Th 90	36.02 40.75 Pa 91	37.36 42.27 U 92	38.65 43.96 Np 93	40.12 45.40 Pu 94	41.53 47.03 Am 95	42.98 48.72 Cm 96	44.47 50.39 Bk 97	45.99 52.18 Cf 98	47.53 53.93 Es 99	49.10 55.69 Fm 100	50.73 57.58 Md 101	52.36 59.35 No 102	54.06 61.28 Lr 103	Actinides 90-103						
12.03 14.77 Lanthanides 57-71	12.65 15.71 La 57	12.97 16.20 Ce 58	13.29 19.70 Pr 59	13.61 17.22 Nd 60	13.95 17.74 Pm 61	14.28 18.28 Sm 62	14.62 18.83 Eu 63	14.96 19.39 Gd 64	15.31 19.97 Tb 65	15.66 20.56 Dy 66	16.02 21.17 Ho 67	16.38 21.79 Er 68	16.74 22.42 Tm 69	17.10 23.09 Yb 70	17.41 23.76 Lu 71								

	$K_{\alpha 1}$ 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

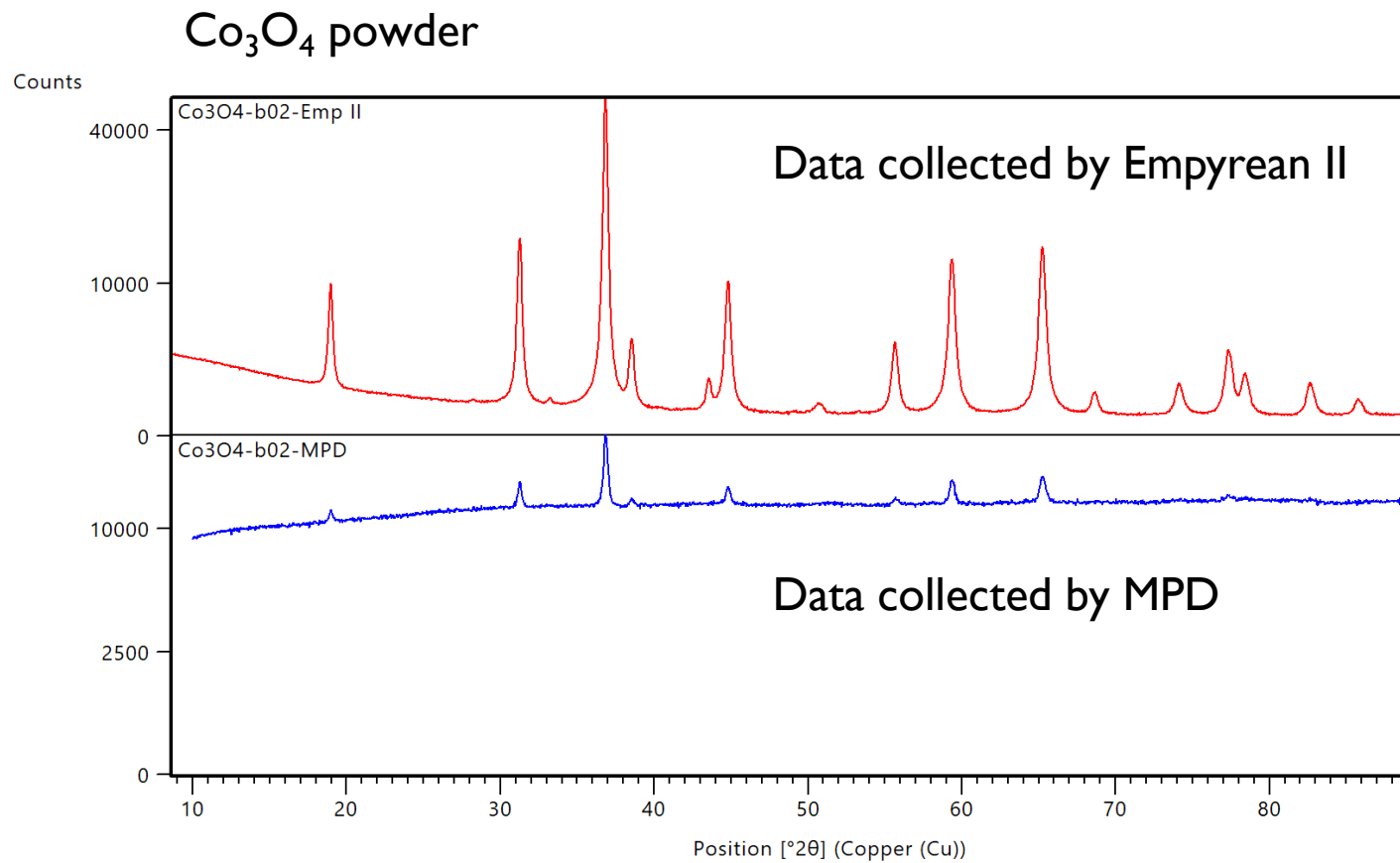
# CASE STUDY I

## FeSi<sub>2</sub> 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?

