In diffraction experiment

- Diffraction lines at $\vartheta = 21.65°$
  $25.22°$
  $37.06°$
  $44.96°$
  $47.56°$

- Powder diffraction experiment.

- $\lambda = 1.5$ Å

Question: Is this FCC, BCC, SC? → All three achievable by a choice of basis on SC {Lattice}

Diffraction occurs between planes of: $d = \dfrac{a}{\sqrt{h^2 + l^2 + k^2}}$

a → Lattice constants

Due to basis: BCC: $h+k+l$ must be even.
FCC: h, k, l all even or all odd.

This formula includes planes without atoms, e.g. (200) in SC. However $n=1$ diffraction from these planes ⇔ $n>1$ for planes w/ atoms.

We set $n=1$ for Bragg's Law when using it. → Higher order diffraction from planes ⇔ to 1st order from others. Prove?

$n\lambda = 2d \sin\Theta$

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$$\lambda = \frac{a}{\sqrt{h^2+l^2+k^2}} 2\sin\theta$$

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+l^2+k^2)$$

By observing this is constant we can instead consider $\frac{\sin^2\theta_i}{\sin^2\theta_j} = \frac{(h^2+k^2+l^2)_i}{(h^2+k^2+l^2)_j}$ for the allowed values of h, k, l from restrictions above.

structure	$h^2+k^2+\ell^2$ sequence								ratios
sc	1_{100}	2_{110}	3_{111}	4_{200}	5_{210}	6_{211}	·	8_{220}	1 : 2 : 3 : 4 : 5 : 6 : 8 : . . .
bcc	·	2	·	4	·	6	·	8	1 : 2 : 3 : 4 : 5 : 6 : 7 : 8 : . . .
fcc	·	·	3	4	·	·	·	8	1 : 4/3 : 8/3 : . . .

For our values we see:

Here, $\sin^2\vartheta = 0.1361, 0.1816, 0.3632, 0.4993, 0.5446$
ratio $= 1.000 : 1.334 : 2.668 : 3.668 : 4.001$

$$1 : \frac{4}{3} : \frac{8}{3} : \frac{11}{3} : 4$$

$$\frac{1}{3} : \frac{4}{3} : \frac{8}{3} : \frac{11}{3} : \frac{12}{3}$$

Which is clearly F.C.C.

Once we have identified the h k l values these correspond to, we can determine a.

Picking (111) being the first plane occupied in FCC we can take,

$$\sin^2 21.65° = \frac{1.5^2}{4a^2} \times 3 \Rightarrow a = 3.52\,Å$$

Which we can identify as nickle from datasets.