

Powder Diffraction

Ron Smith

aided by:

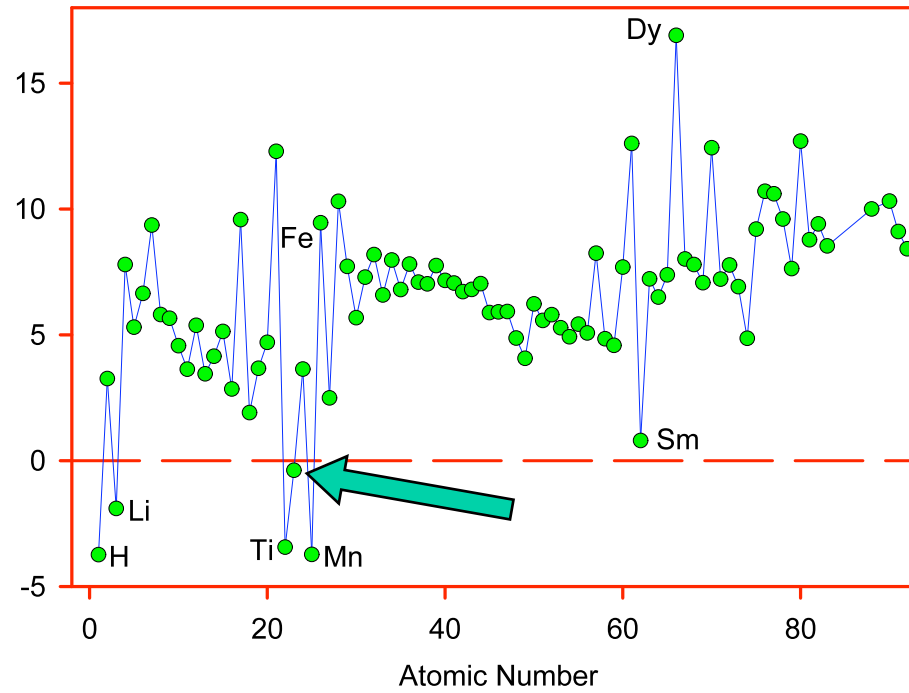
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Practical:

- Data collection on Polaris and GEM
(high flux, medium resolution powder diffractometers)
- Sample loading (*vanadium* cans)
- Data collection at room temperature
- Variable temperature measurements in a cryostat

Why vanadium?

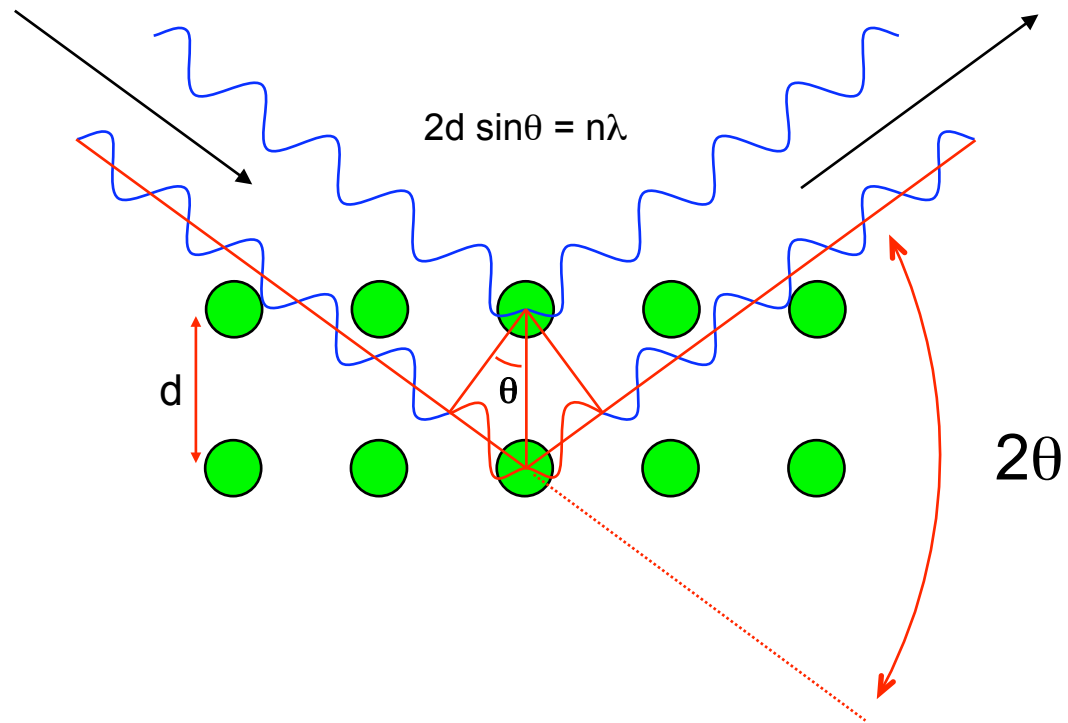


$$b = -0.38 \text{ fm}$$

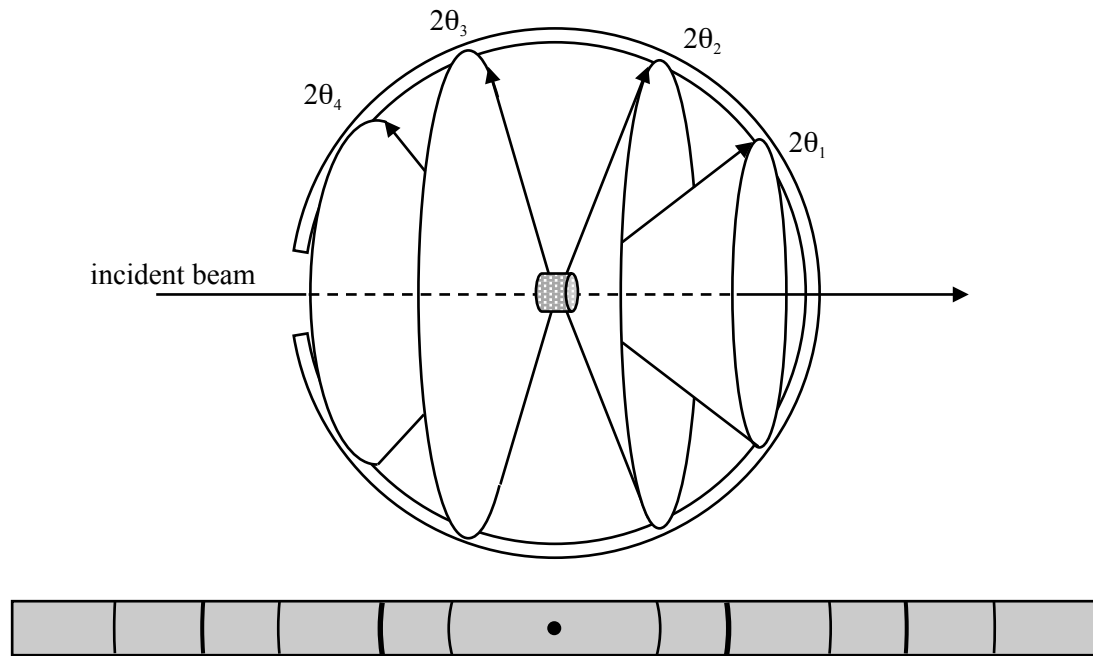
Worksheets

- data normalisation
- indexing
(structure factors and systematic absences)
- identification of unknown materials
- resolution
- Rietveld refinement
 - GSAS Instrument Parameter File
 - Magnetic Neutron Diffraction

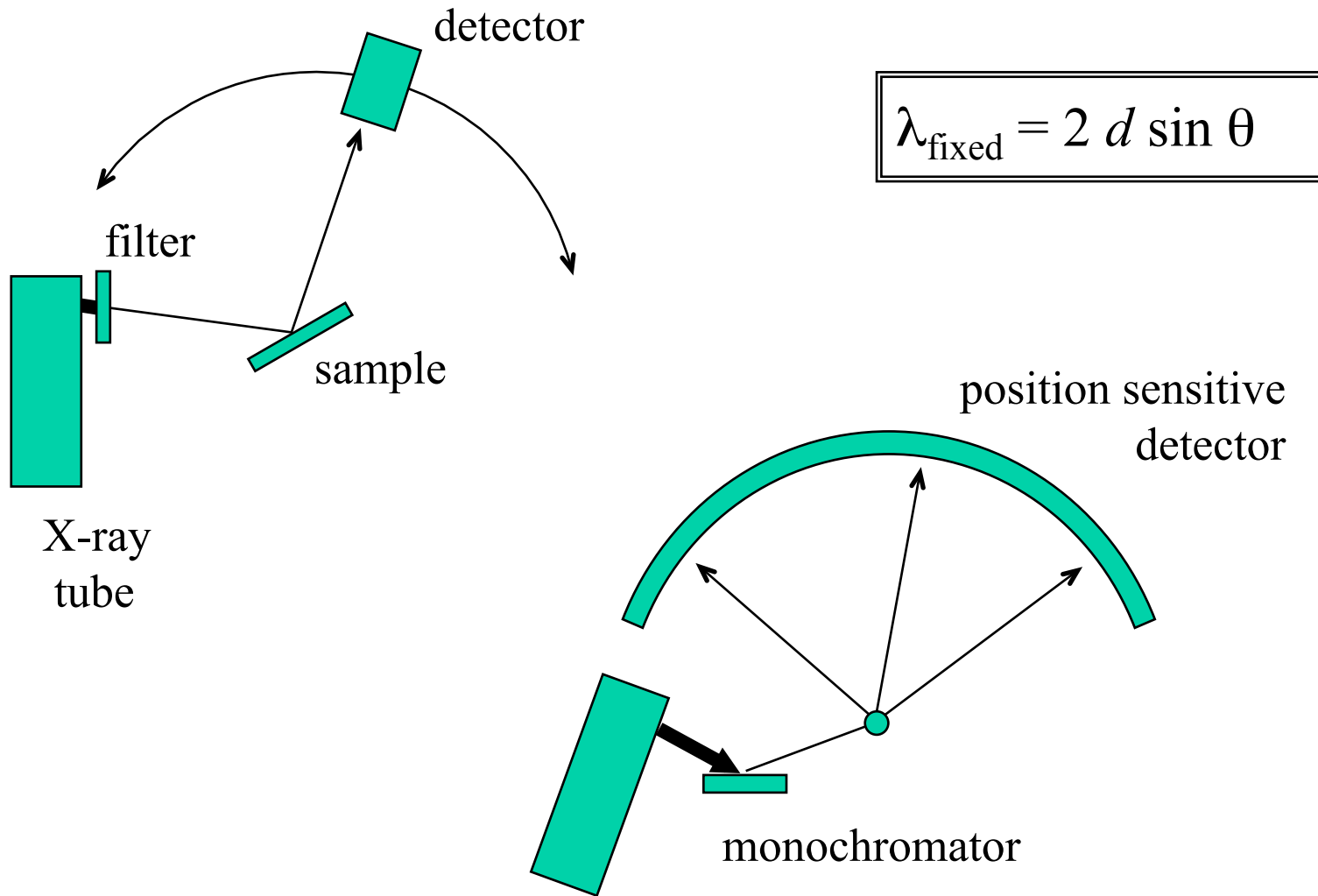
Bragg's Law



diffracted beam at angle 2θ to transmitted beam



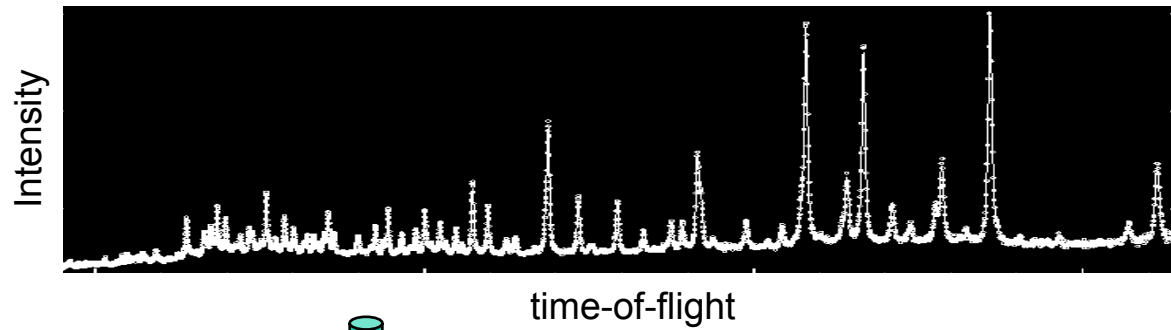
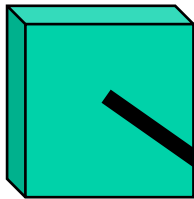
Data collection: constant wavelength



Time-of-flight diffraction: no moving parts

$$\lambda = 2 d \sin \theta_{\text{fixed}}$$

neutron
source



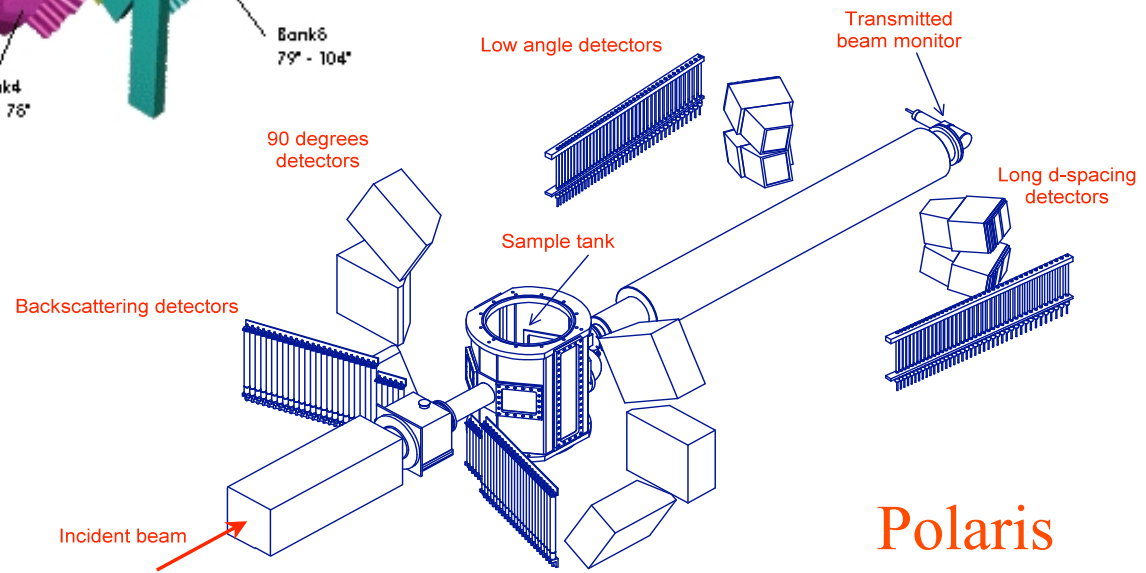
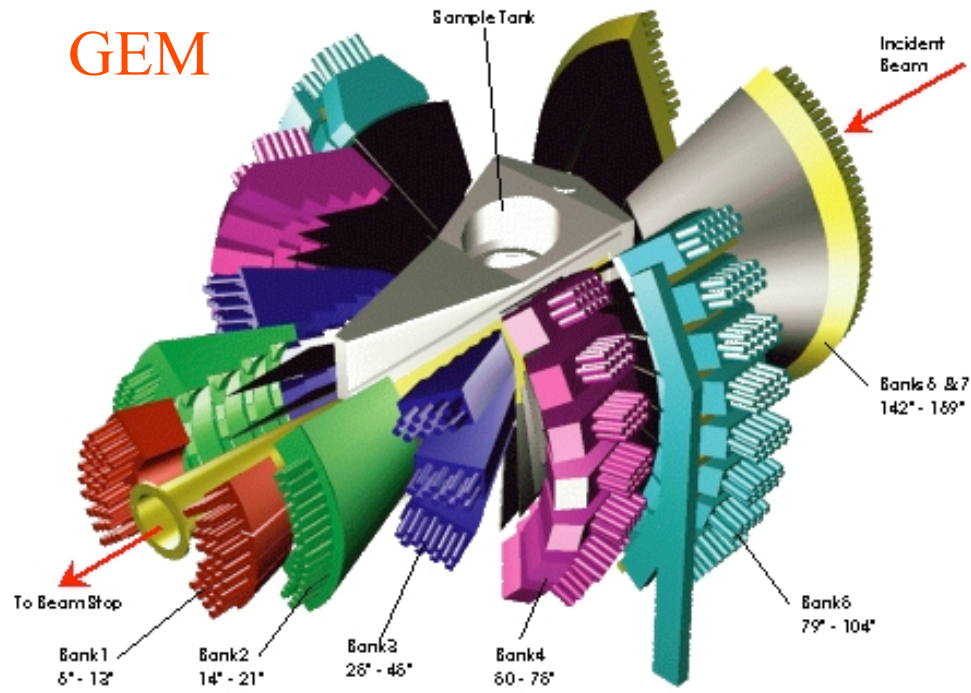
detector



sample



GEM



Polaris

Normalisation

- constant λ source: "fixed" incident intensity
- pulsed source: incident intensity varies with neutron energy - wavelength dependent corrections (absorption and multiple scattering)

Worksheets: Practical, Exercises, Questions

- powder diffraction data collection
 - nickel powder (index)
 - two "unknown" materials (index and identify)
- algebraic equation manipulation
 - indexing and calibration
 - resolution
 - structure factor calculation (systematic absences)
- a "real" experiment
 - magnetic neutron diffraction
- Rietveld refinement
 - prepare instrument parameter file
 - magnetic structure refinement

