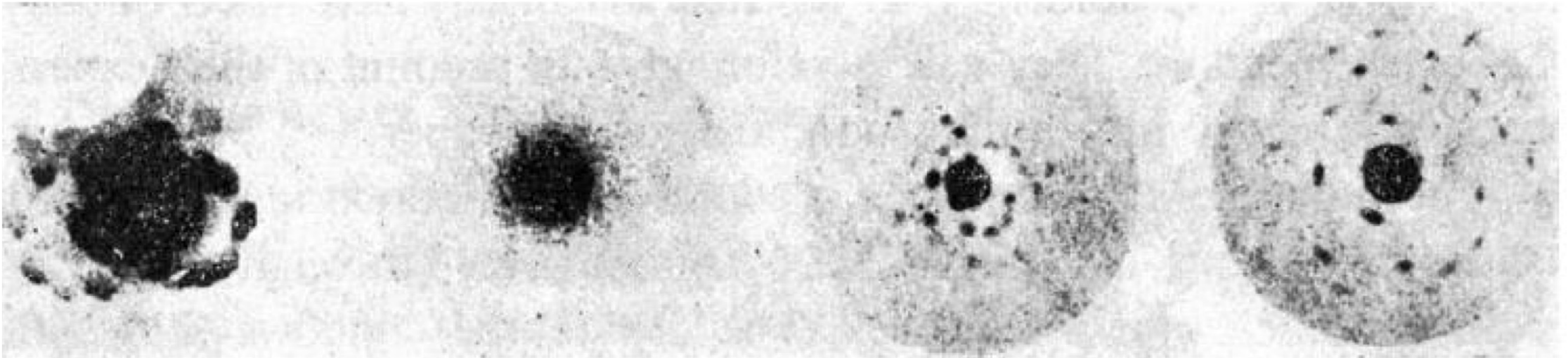


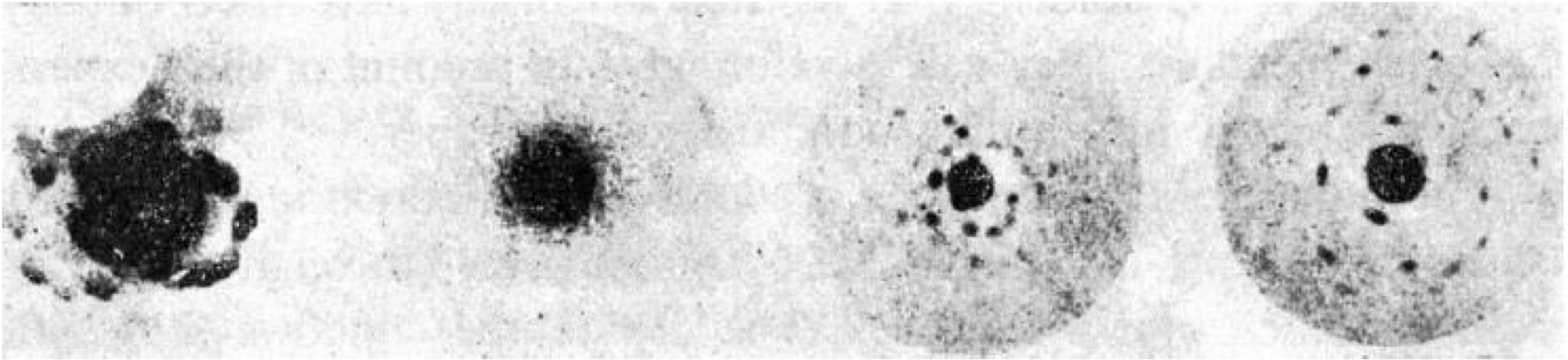
Thin film characterization

Von Laue - Theoretical physicist claiming X-Rays are waves

Elements of XRD Analysis



First X-Ray pattern by Walter Friedrich and Paul Knipping on ZnS, 1912



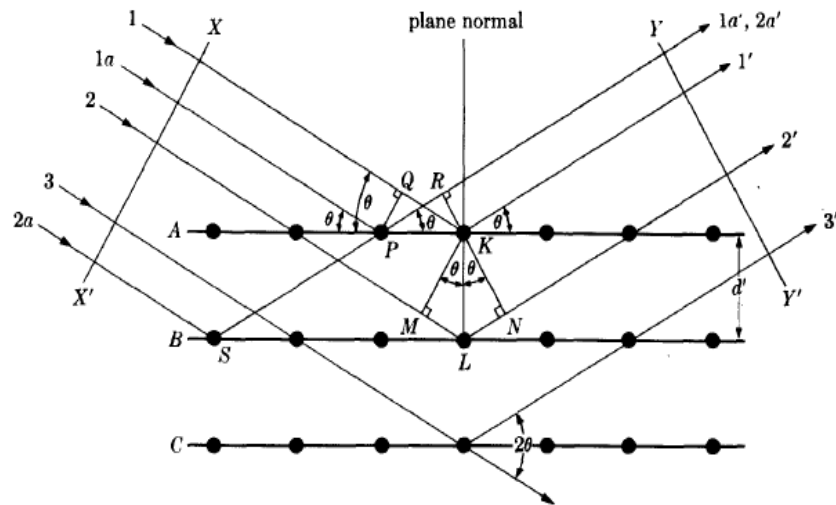
Laue: ZnS crystal is an infinite collection of cubes with Zn and S occupying alternate columns!

L. and W. Bragg: Look there are spots which are not so bright! – There should also be atoms on the walls of the cubes!

H. Armstrong: 'This is repugnant to sense! - Absurd to nth degree. It seems you will say that the rock salt does not contain molecules of 'NaCl' but a simple extension of N-Cl atoms?

Xray study components:

$$\lambda = 2d_{nh,nk,nl} \sin \theta$$



$$\text{Intensity } I = |F|^2 p \left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) e^{-2M}$$

$$F = \sum_1^n f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

Atomic scattering factor (f_n) and phase interference

Intensity along Bragg's angle $I \propto FF^*$

Other factors:

Polarization

Multiplicity

Lorentz

Absorption

Temperature

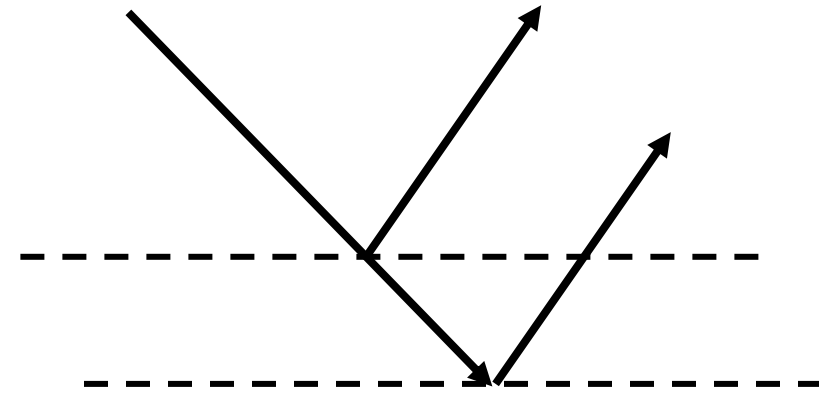
Somewhere around two-dozen nobel prizes for work on X-Rays. Venki Ramakrishnan the latest among them for structure of R

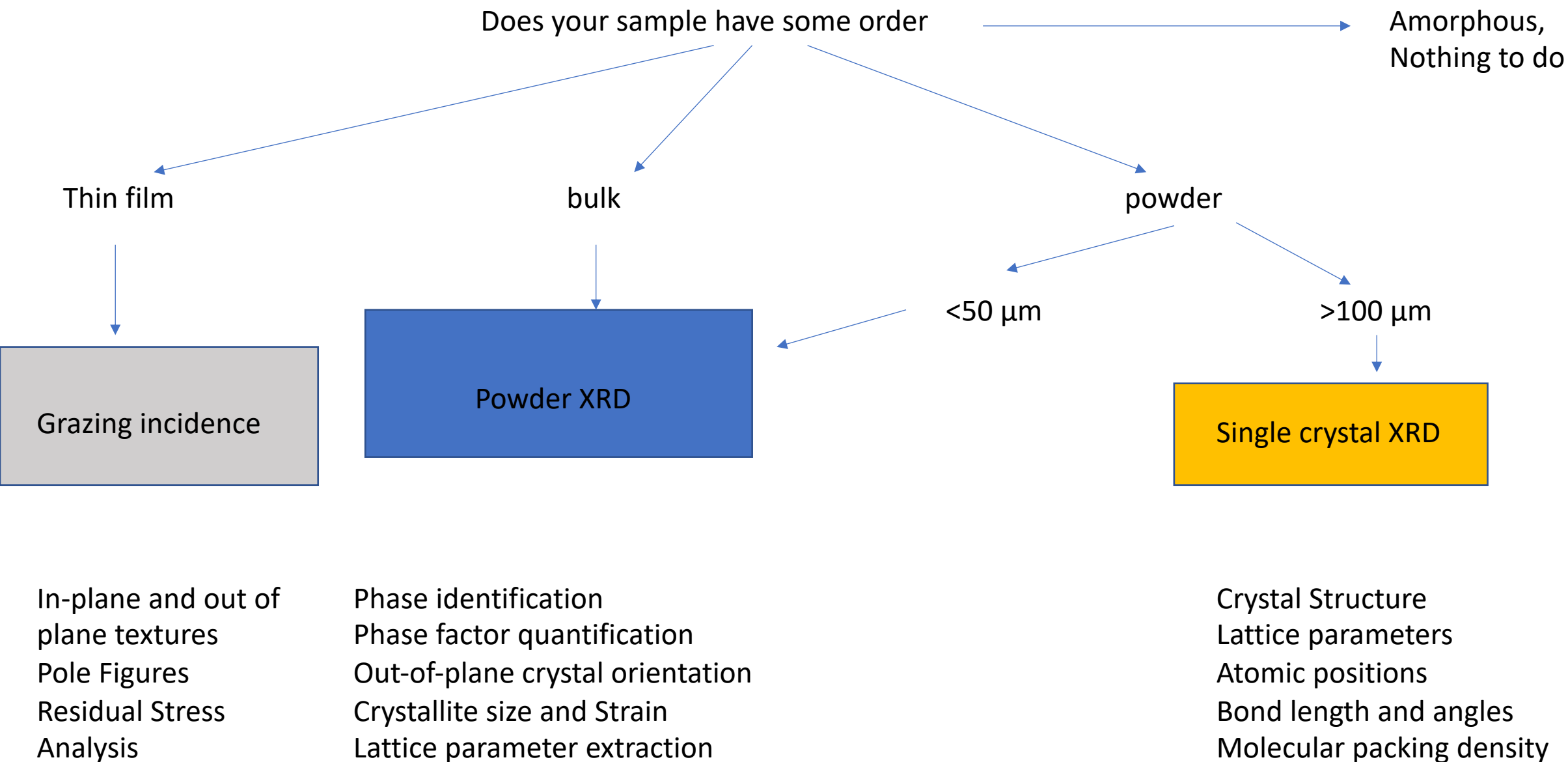
The Idea

- In crystals with atomic ordering,

Radiations reflected by independent planes have path differences proportional to the interplanar spacing!

If the path difference is integer multiple of wavelength, then 'diffraction' information can be used to inspect the interplanar spacing!



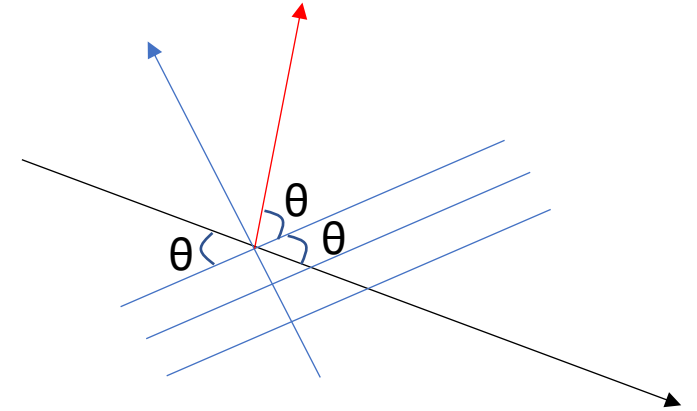


Experimental XRD

Bragg's condition is necessary!

The incident beam is reflected at some plane normal!

If θ is the angle between incident ray with the planes, the diffracted beams are always at 2θ to the transmitted beam.



How do we now construct a device to identify all the planes in the system ?

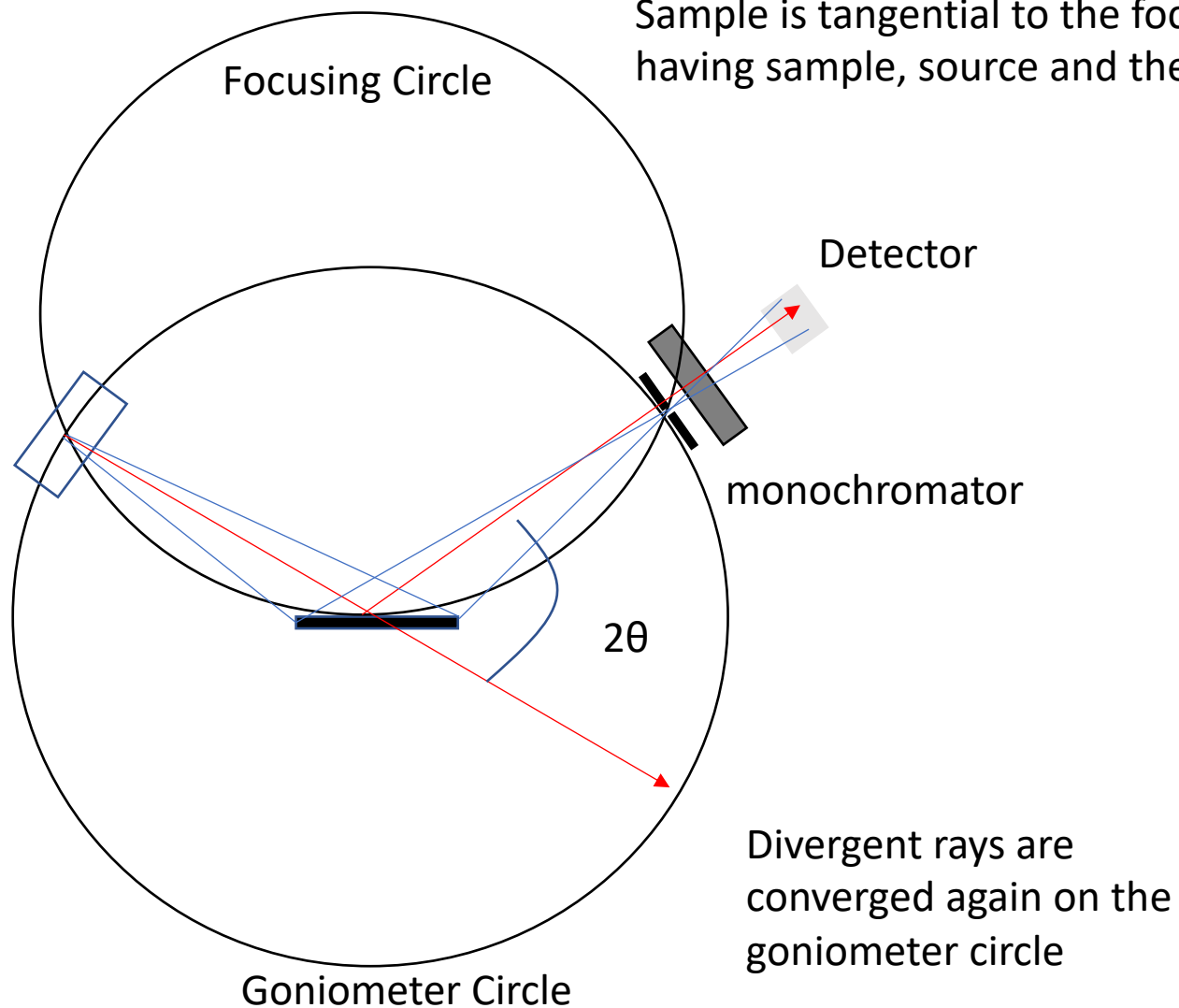
1. Set the source and detector always at Bragg's condition and look for the beam
2. Keep the source constant and rotate a crystal to expose all the planes
3. Send in a broad band X-Ray source and record on a photographic plate!

Geometries of measurement

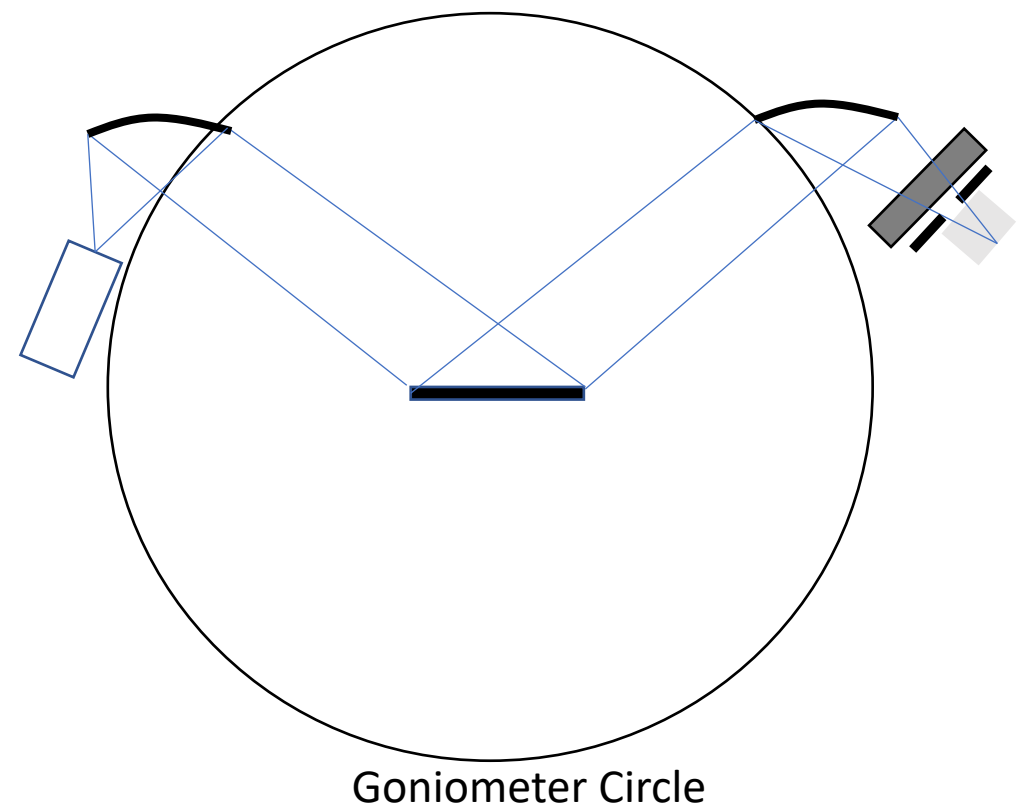
The source and the detector moves on the goniometer circle

Bragg-Brentano

Sample is tangential to the focusing circle having sample, source and the detector slits



Parallel beam

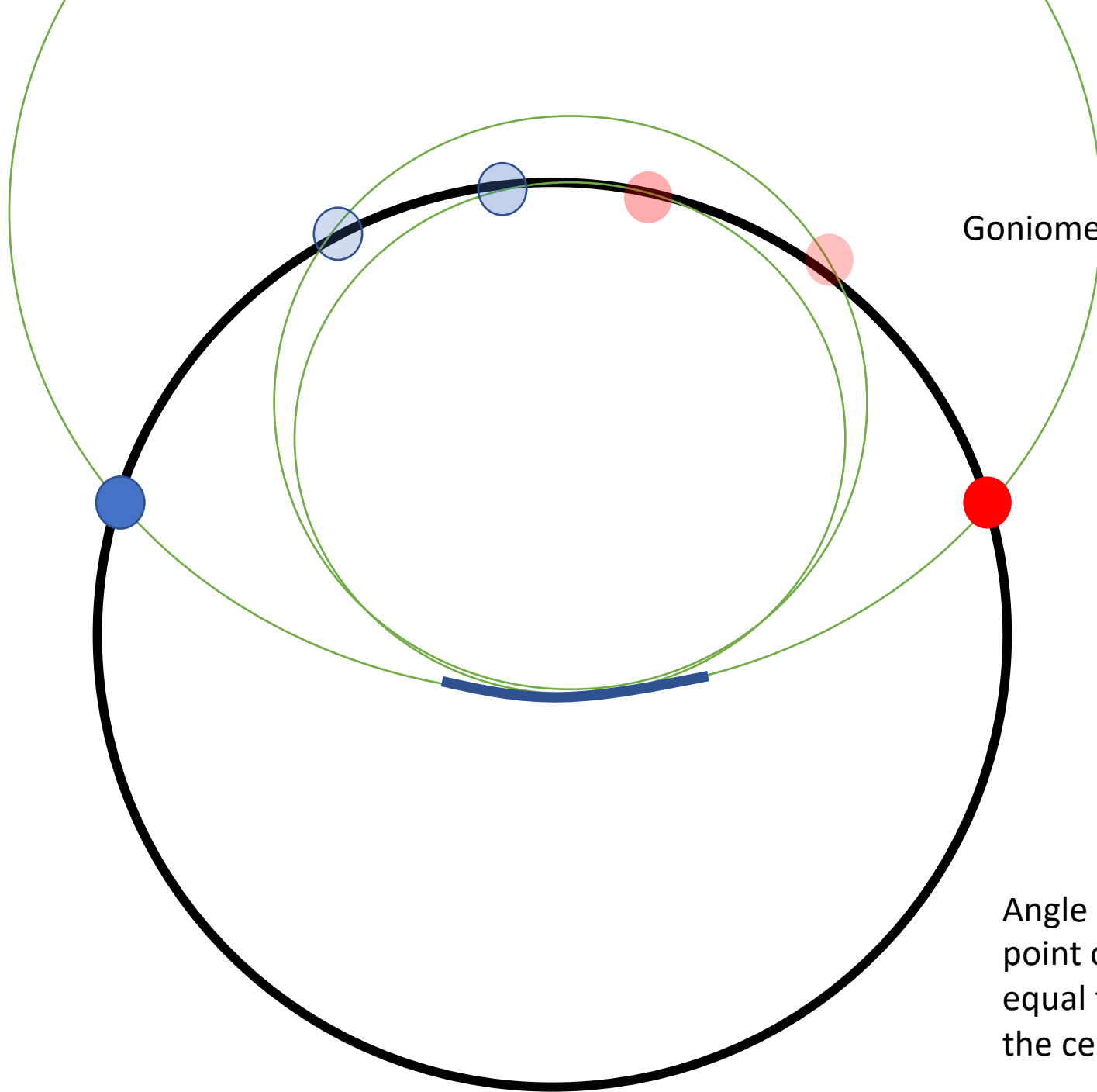


Parafocusing

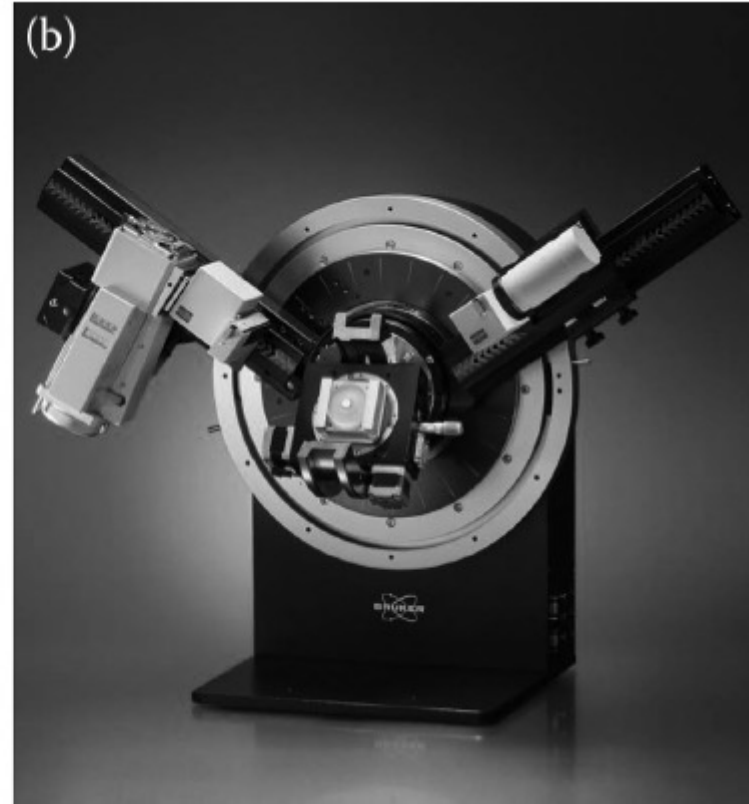
Goniometer Circle

The incident beam though
diverging subtends closely
similar angles to the entire
sample

Angle subtended by an arc on any
point on the remaining circle is
equal to half that it subtends at
the center



Typical commercial X-Ray diffractometer



Parts of a typical X-Ray diffractometer

- X-Ray source
- Monochromators
- Ray optics
- X-Ray detectors
- Stage holders

