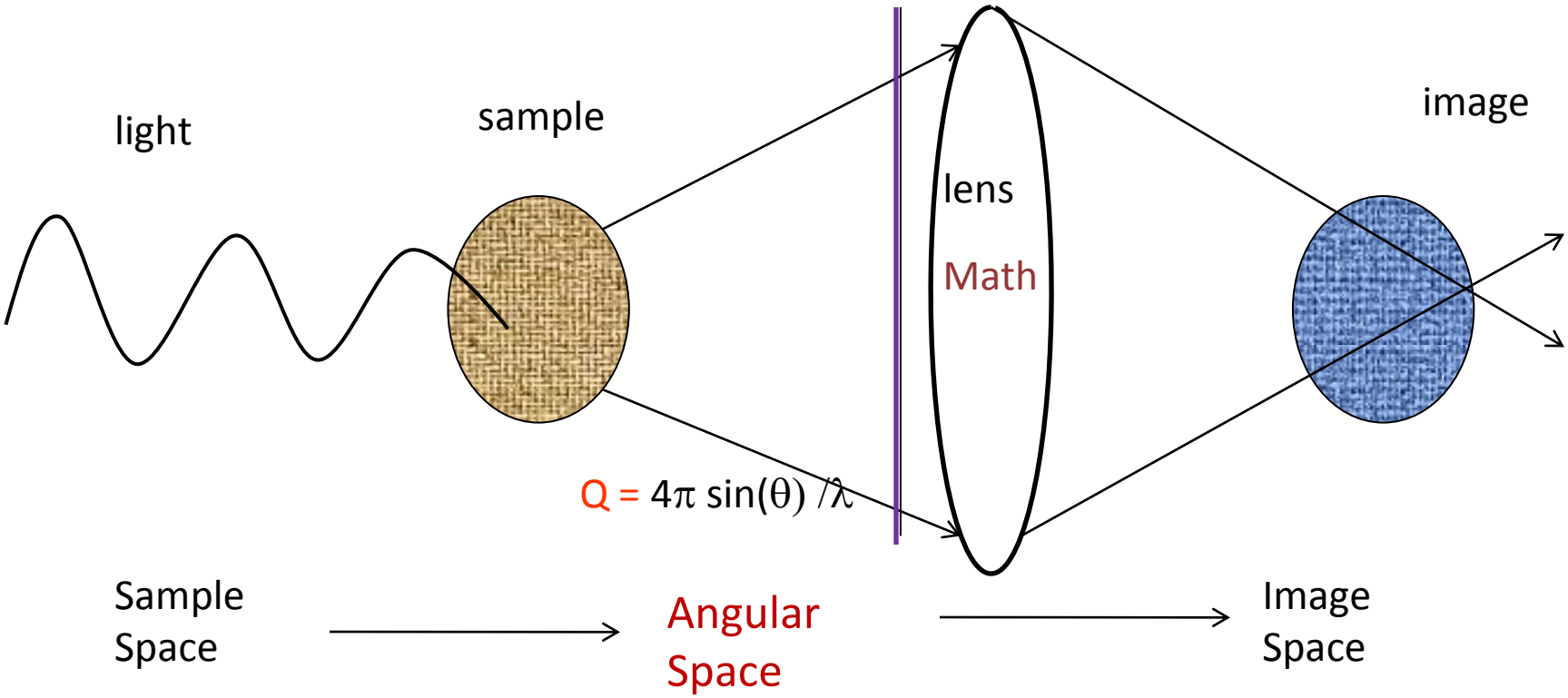
Introduction to Reciprocal Space

7th X-ray Scattering School

Apurva Mehta

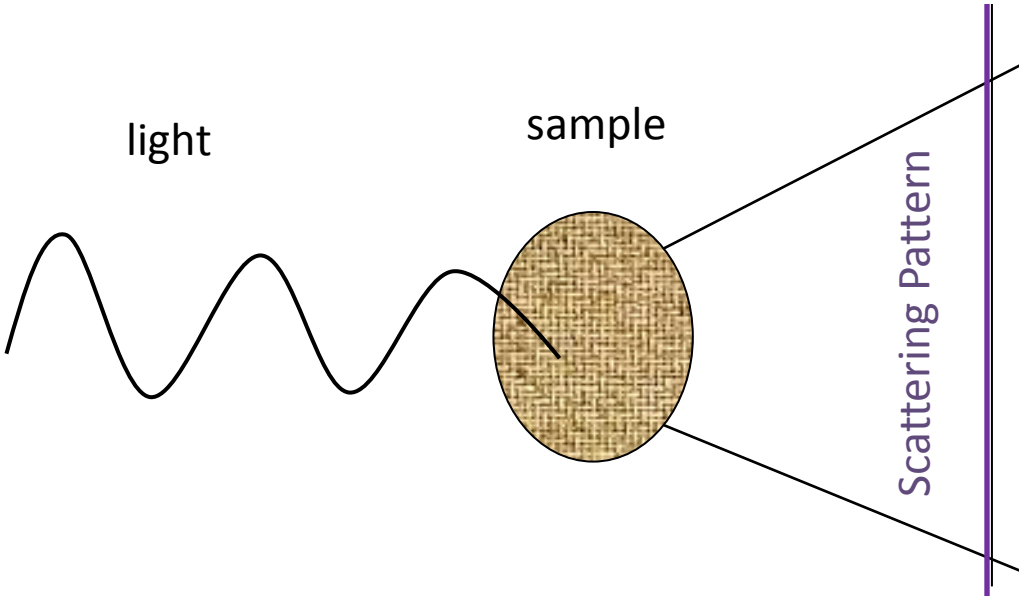
U.S. DEPARTMENT OF ENERGY
Office of Science
SSRL
SLAC NATIONAL ACCELERATOR LABORATORY

Scattering Physics



Can we create the image without a lens?

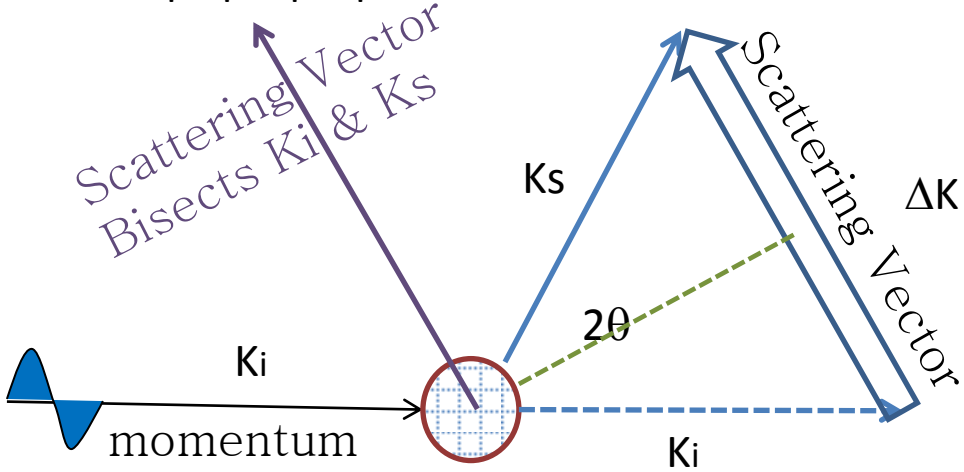
Lensless Imaging



Sample Space → Angular Space

Scattering Physics

Elastic Scattering → $|K_i| = |K_s|$



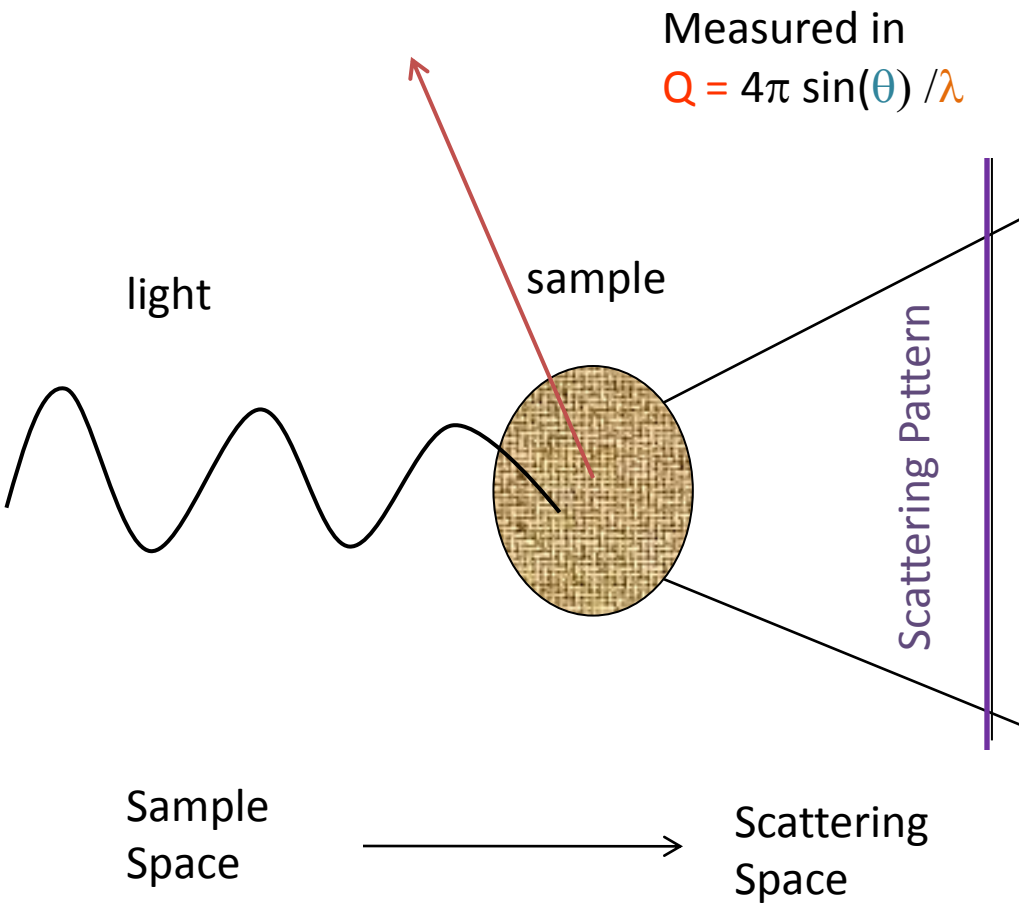
$\Delta K = Q =$ momentum transfer

$\Delta K = Q = 2 * K_i * \sin(\theta)$

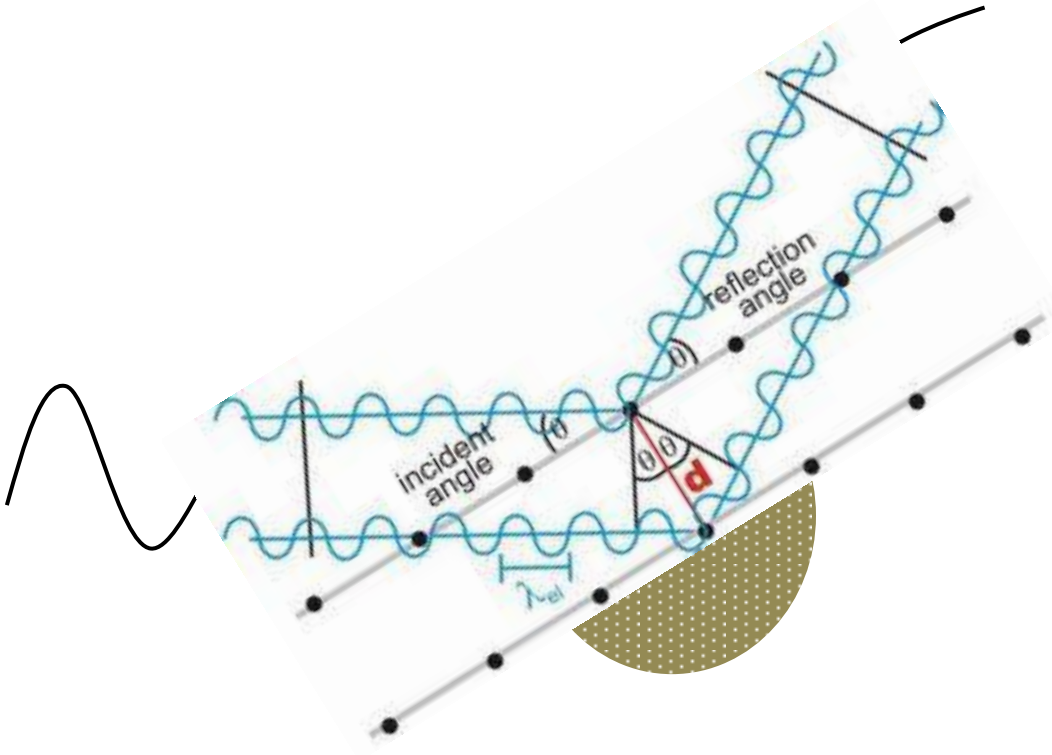
$K_i = 2\pi/\lambda$

$$\boxed{Q = 4\pi\sin(\theta)/\lambda}$$

Lensless Imaging

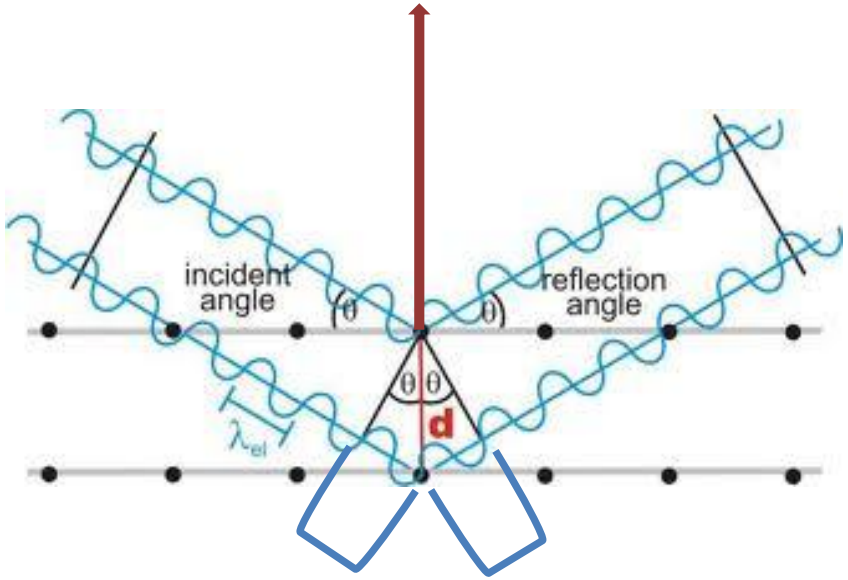


Bragg's Law

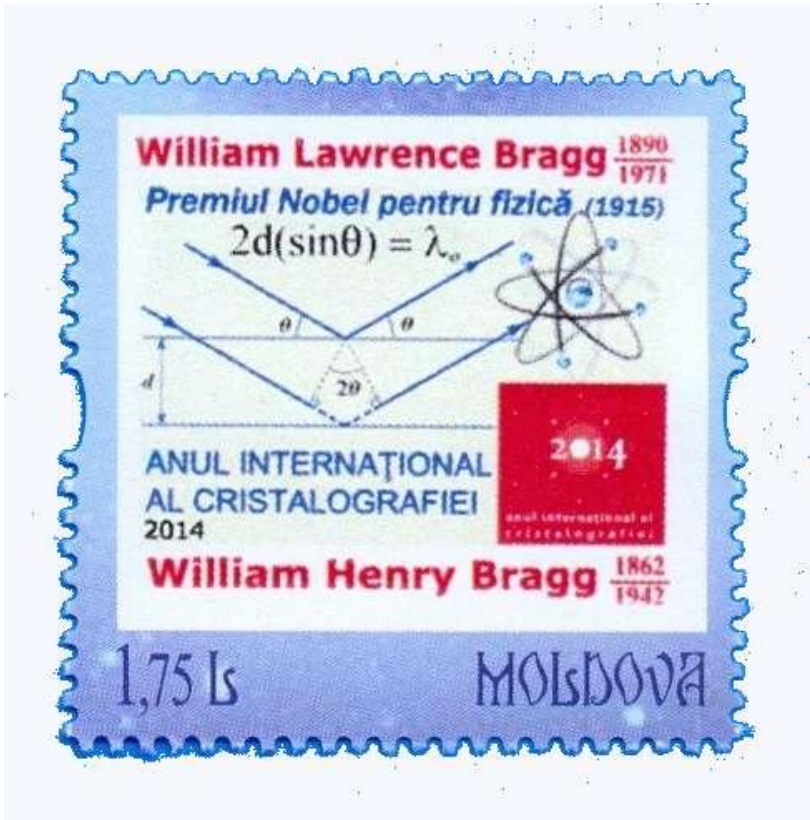


Bragg's Law

Q has magnitude and direction



Proposed in 1912-1913
Nobel Price in Physics - 1915



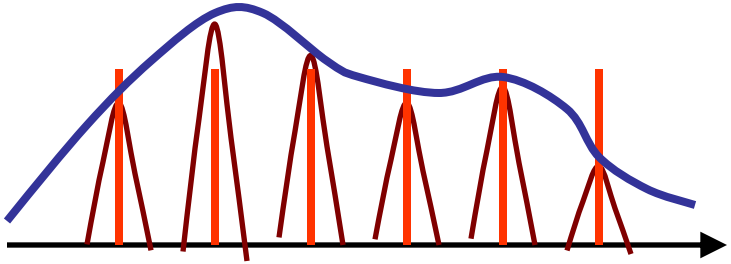
$$2d\sin(\theta) = \lambda$$

$Q = 4\pi\sin(\theta)/\lambda$ → $Q = 4\pi\sin(\theta)/\lambda = 2\pi/d$

$$|Q| = 2\pi/d$$

2014 – International year of Crystallography

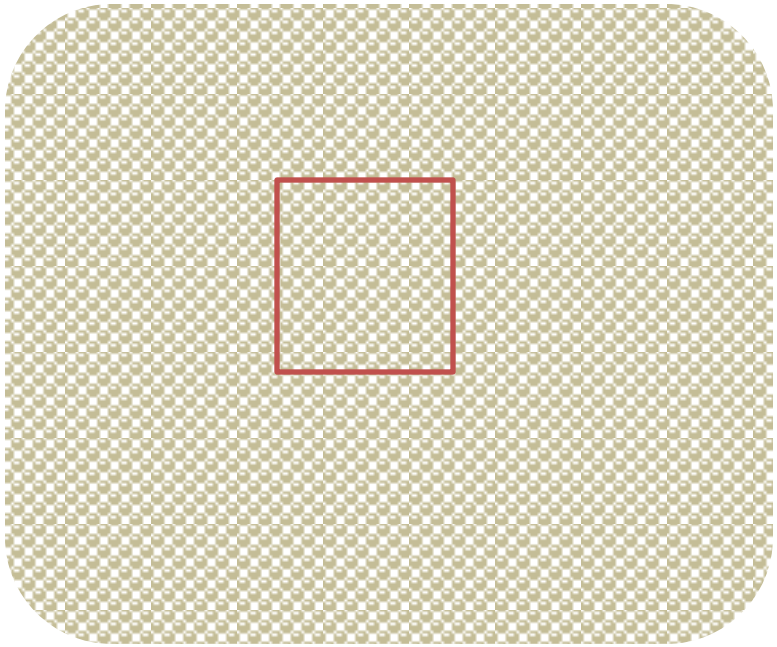
Bragg's Law Tells Us



- About the Position of the scattering peaks
- But not the Direction
- And not its Intensity
- Nor its Width

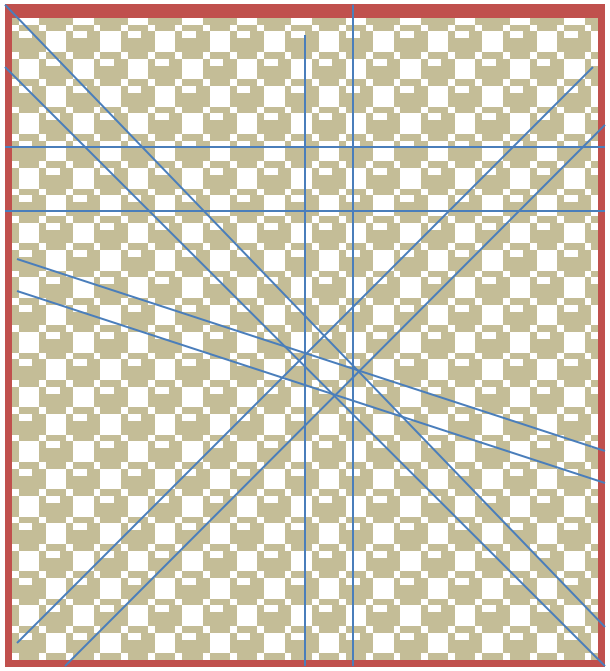
Need to go beyond Bragg's Law

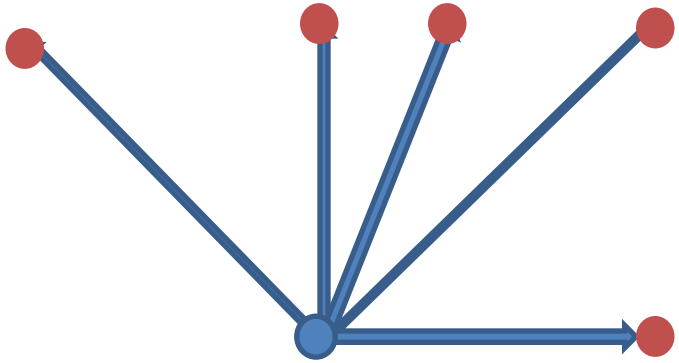
Bragg Planes



Bragg Planes

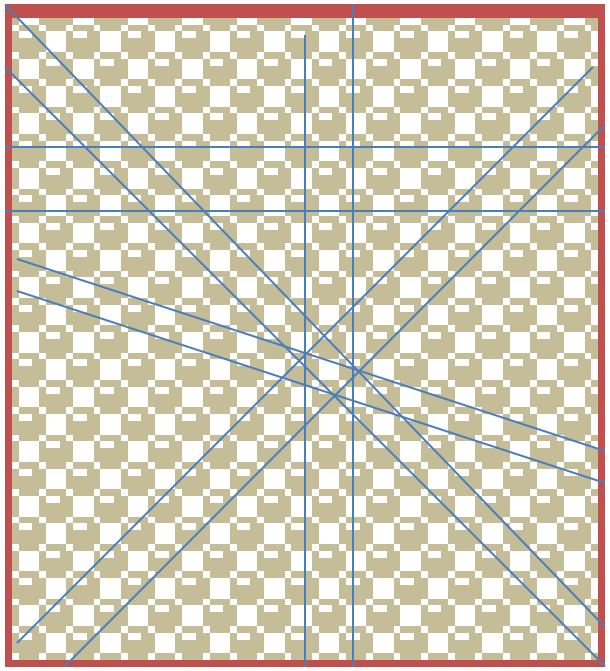
$|Q| = 2\pi/d$

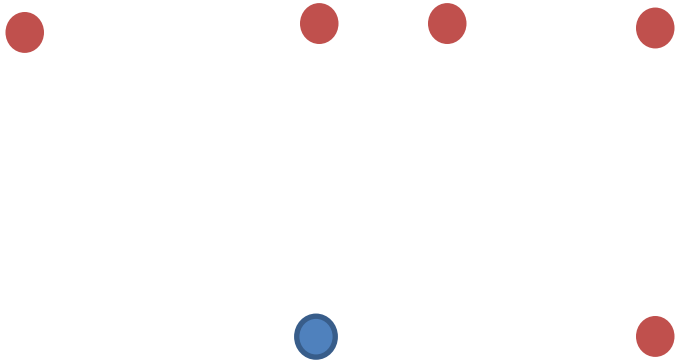




Bragg Planes

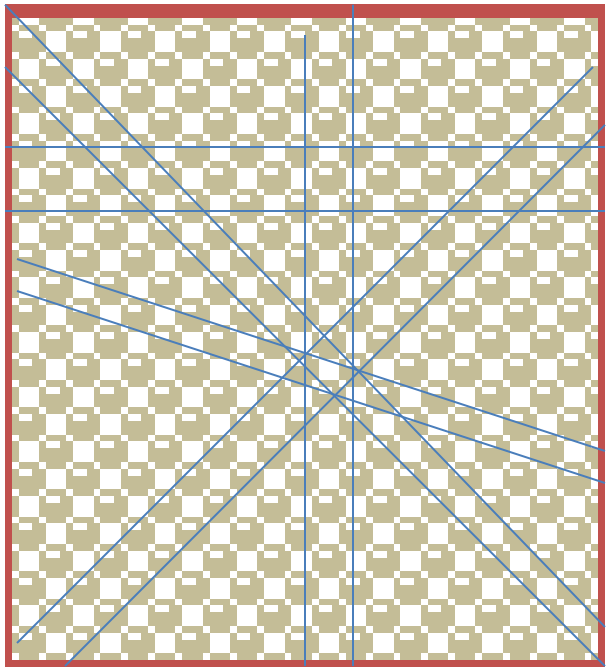
$|Q| = 2\pi/d$

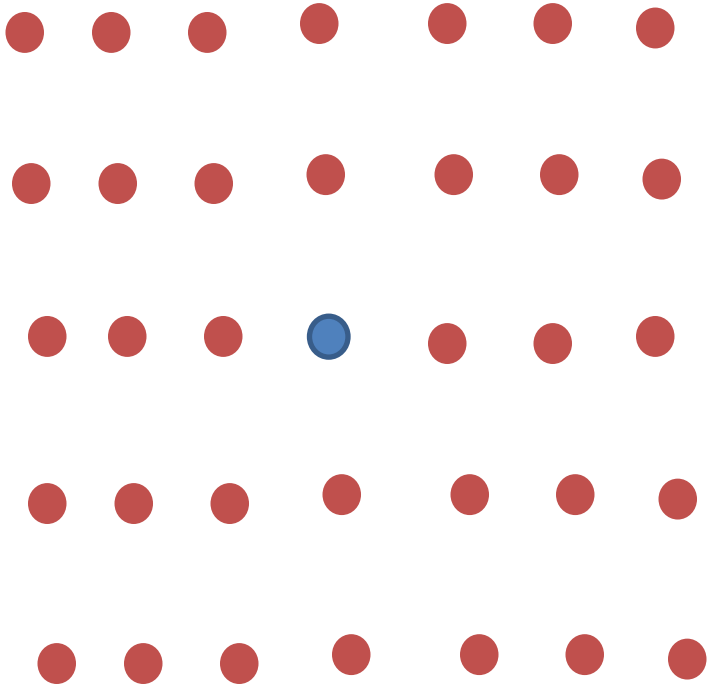




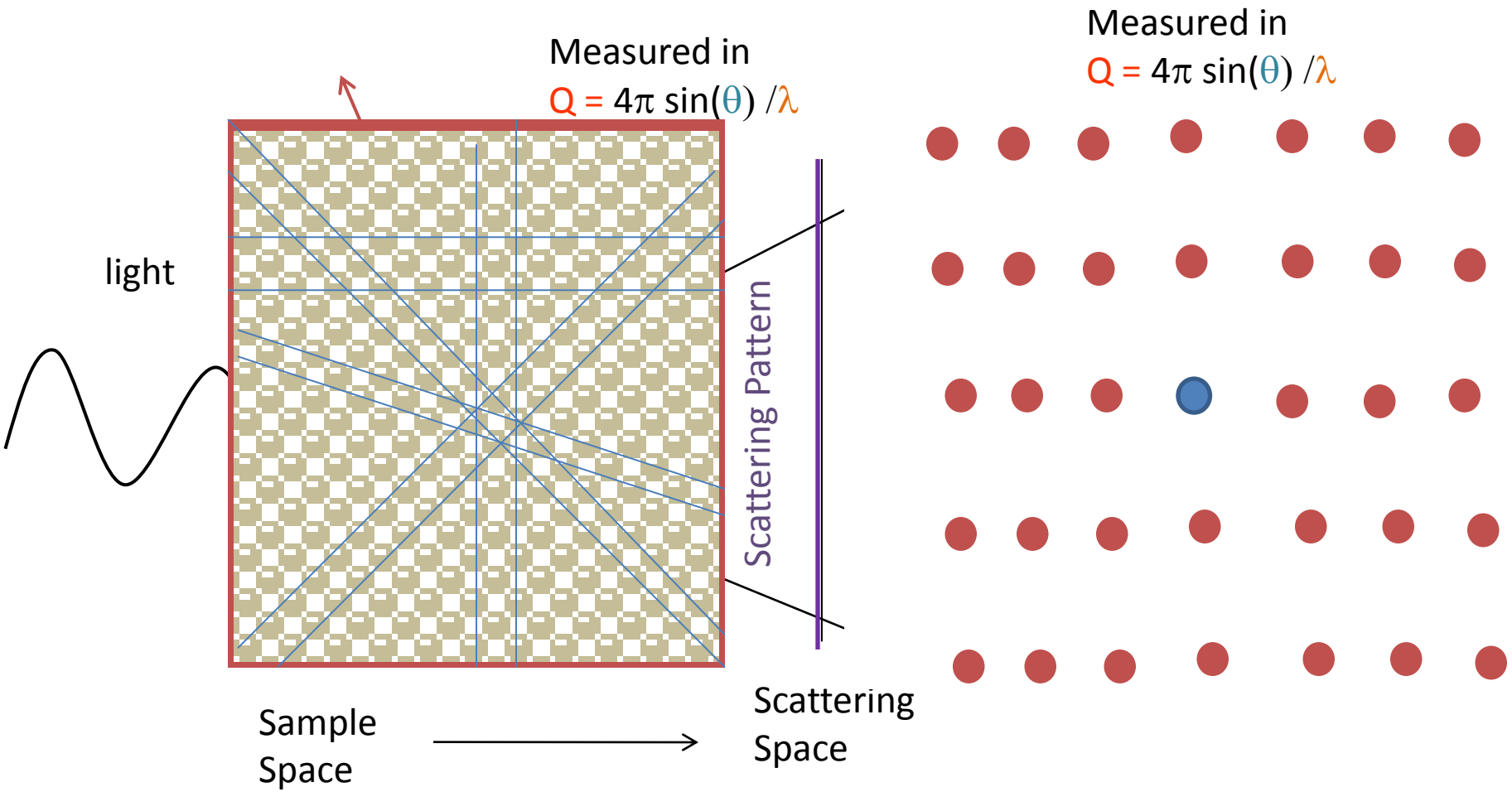
Reciprocal Lattice

$|Q| = 2\pi/d$





Scattering Physics



Real Space Lattice

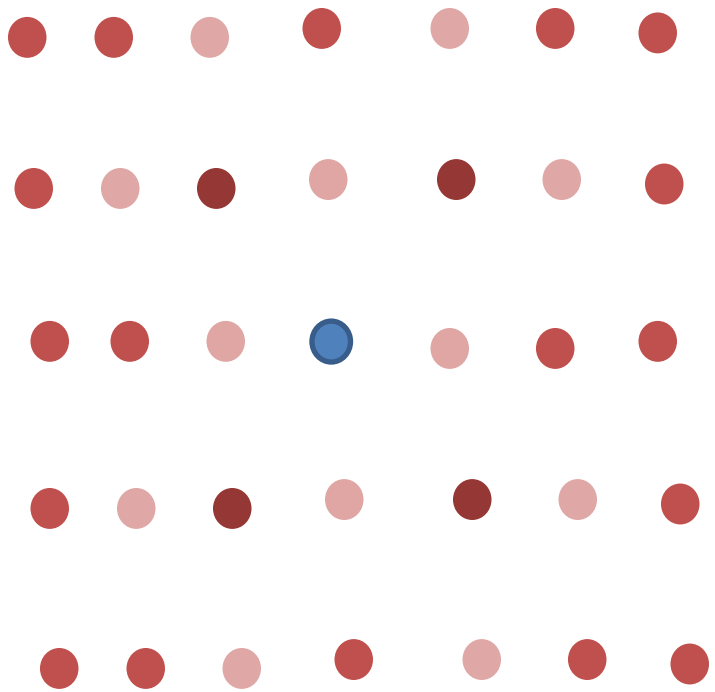
Reciprocal (Space) Lattice

Scattering Physics

- Reciprical Lattice Points
  - Have Position
  - Direction
  - Intensity
  - Width

Measured in

$Q = 4\pi \sin(\theta) / \lambda$

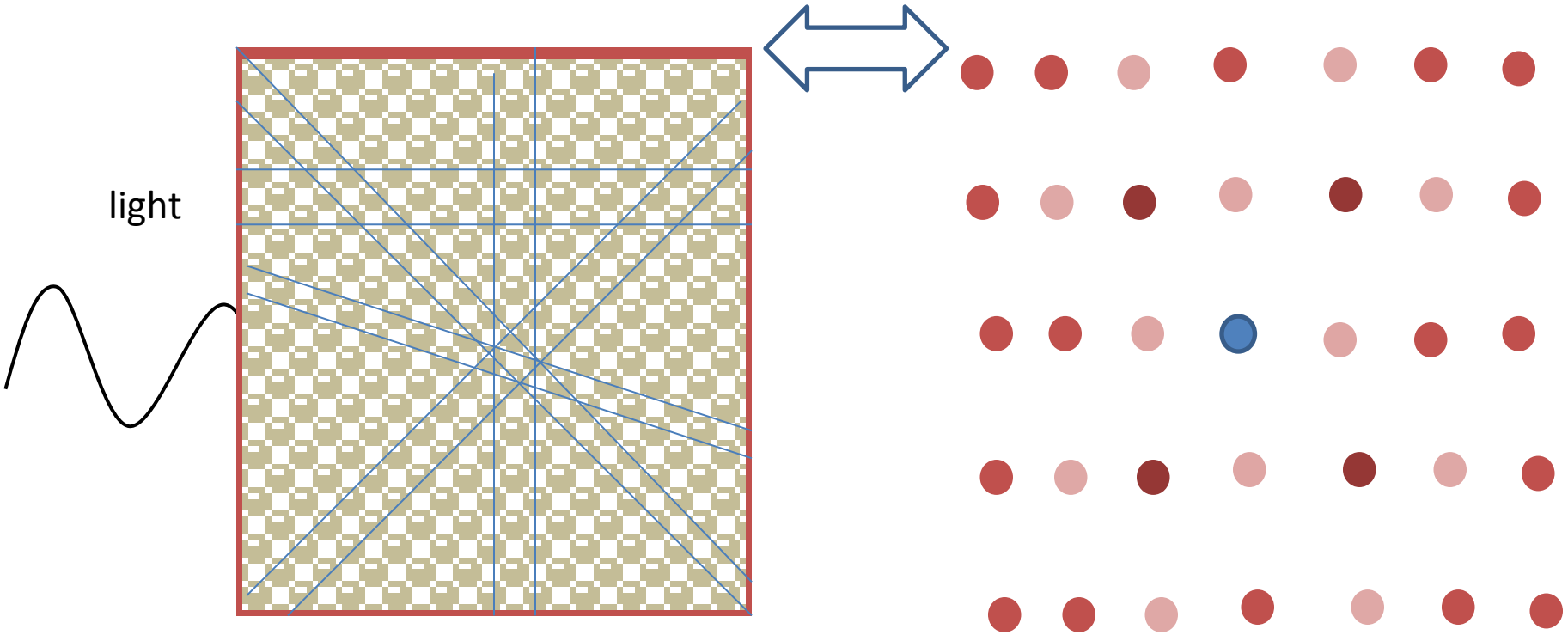


Real Space Lattice

Reciprocal (Space) Lattice

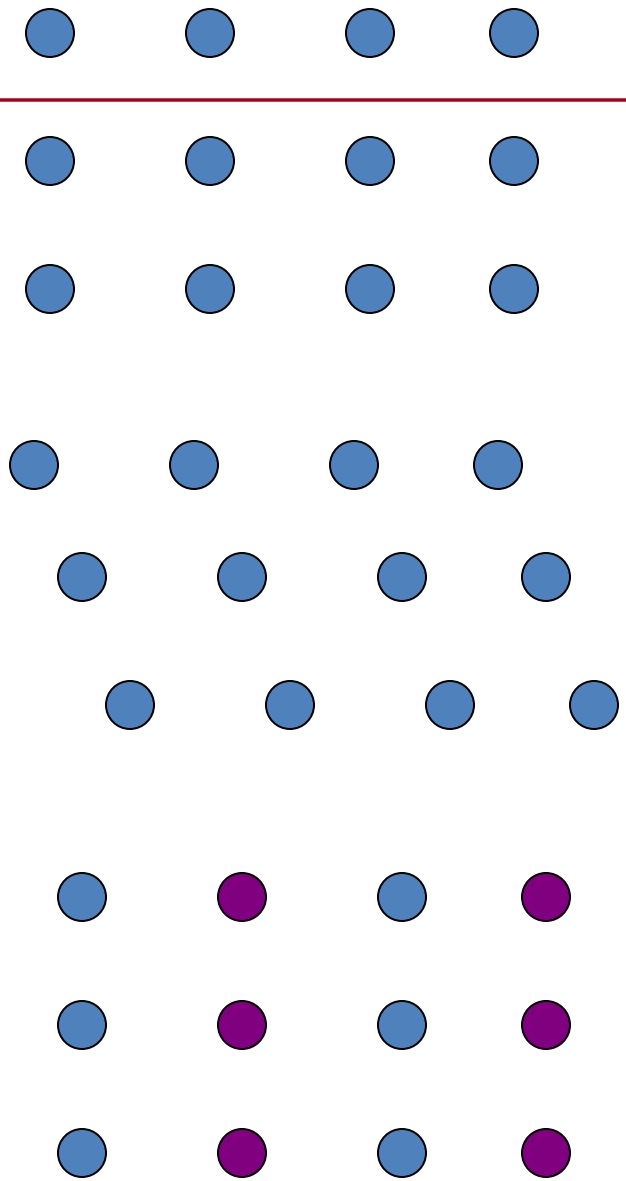
Scattering Physics

Fourier Transform

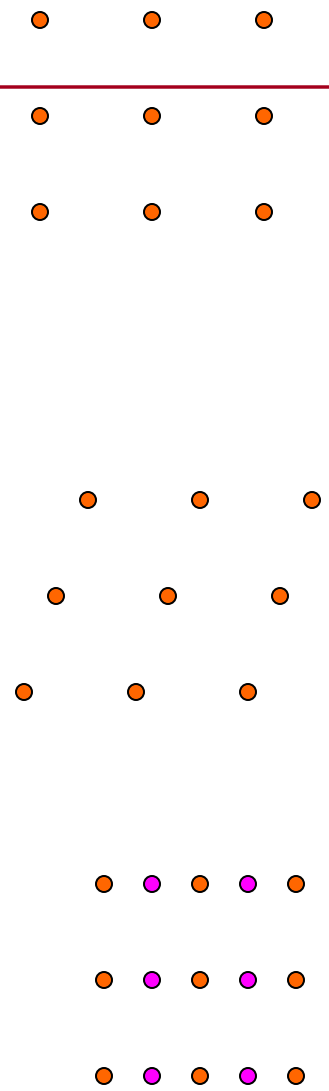


Real Space Lattice

Reciprocal (Space) Lattice

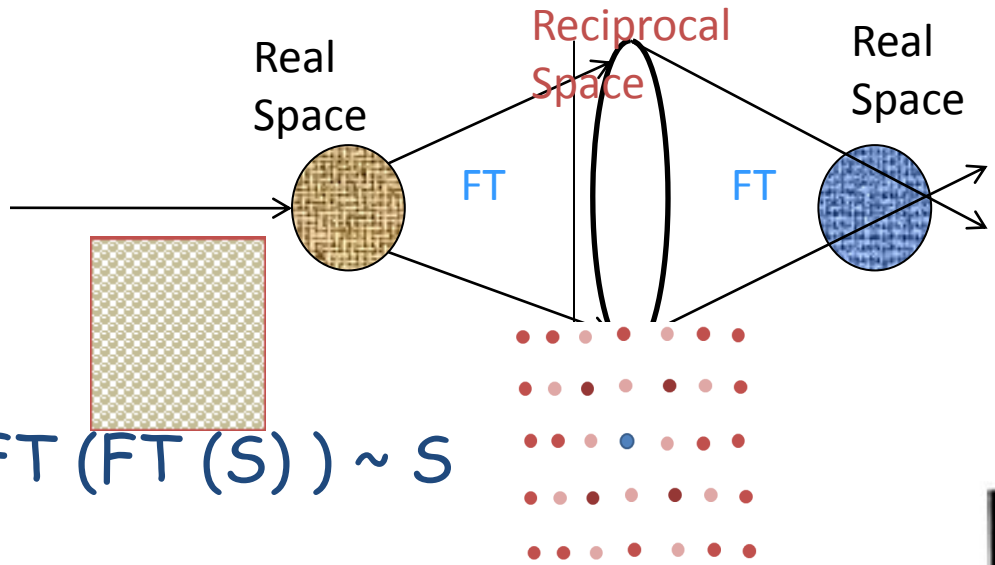


Real Space

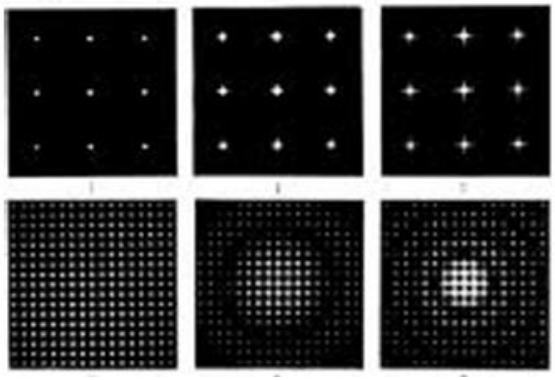


Reciprocal Space

Recap



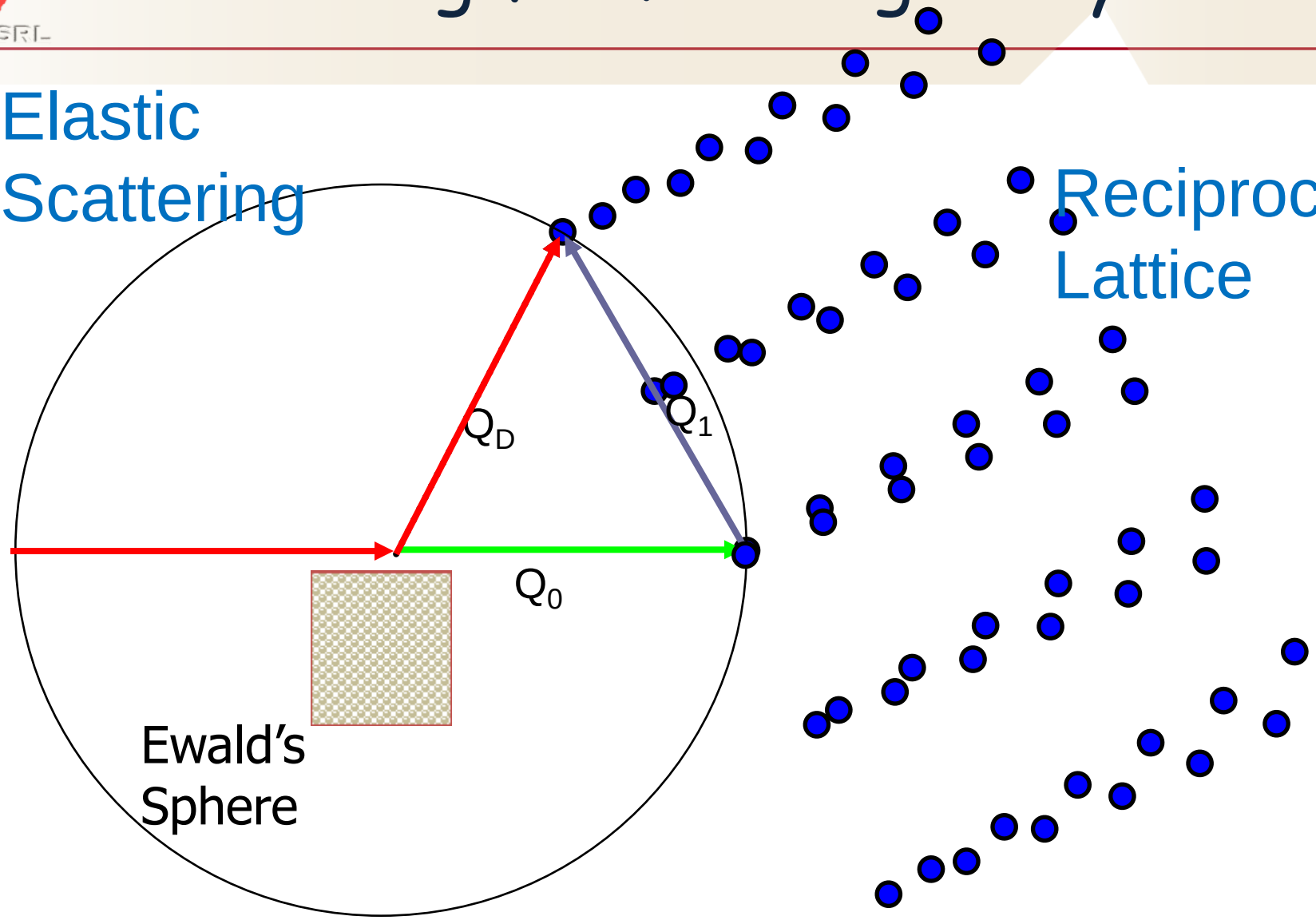
- 1: FT (FT (S)) ~ S
- 2: FT (large) ~ 1/large ➔ small
  - Rec Sp (large) ➔ small
- 3: FT (periodic fn) ~ periodic
  - Rec Sp (periodic Real Sp) ~ periodic



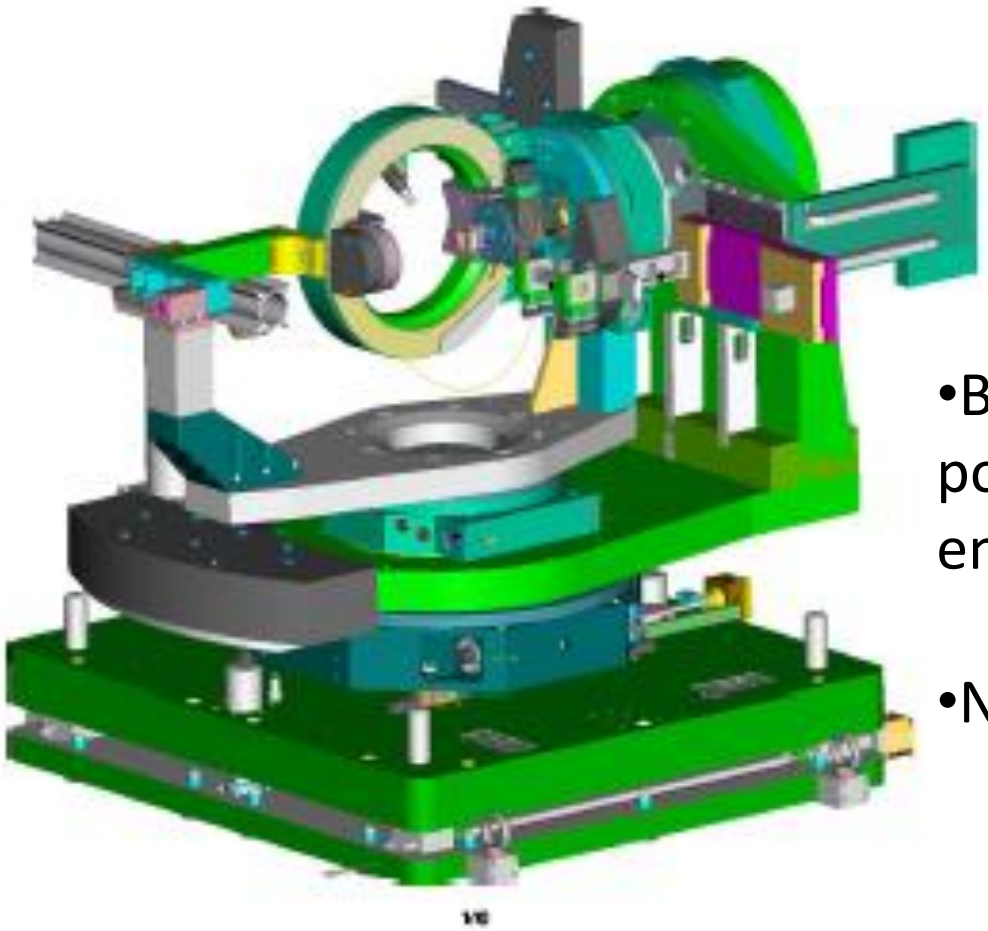
Sailing Through Reciprocal Space

Scattering from a Single Crystal

Elastic Scattering



Multi-circle diffractometer

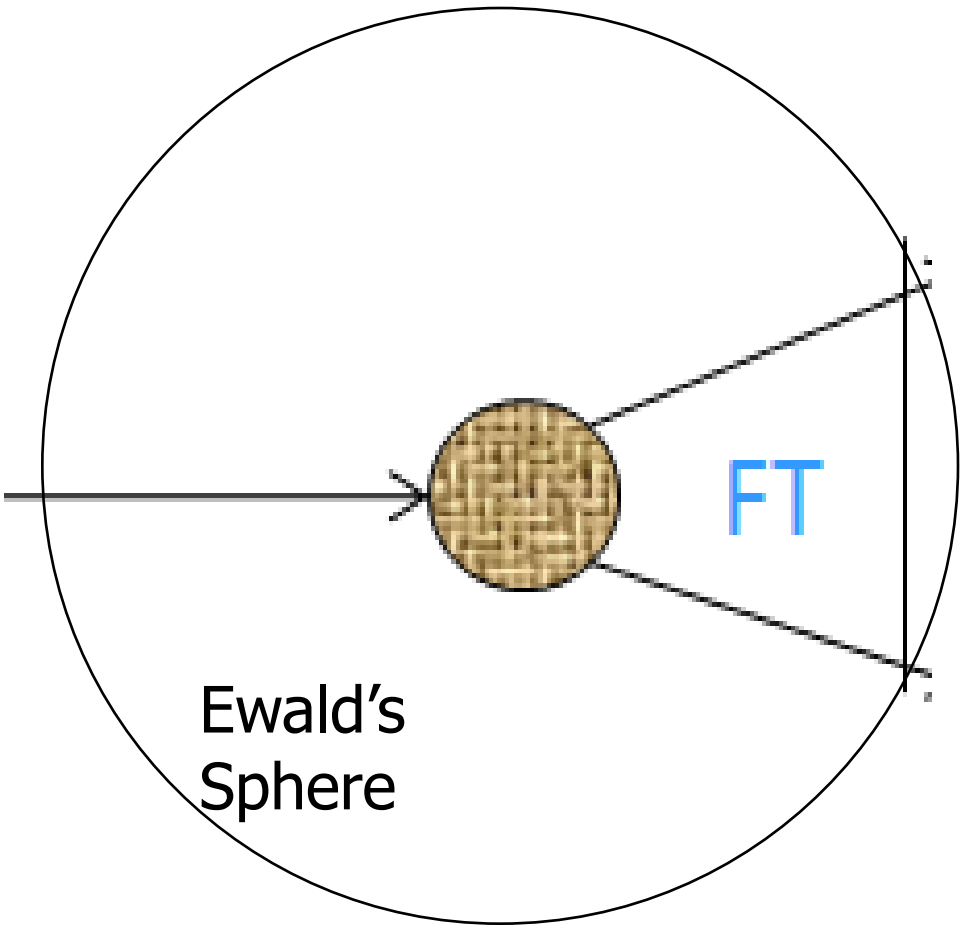


- Need at least
  - 2 angles for the sample
  - 1 for the detector

- But often more for ease, polarization control, environmental chambers

- New Diffractometer @7-2
  - 4 angles for the sample
  - 2 for the detector

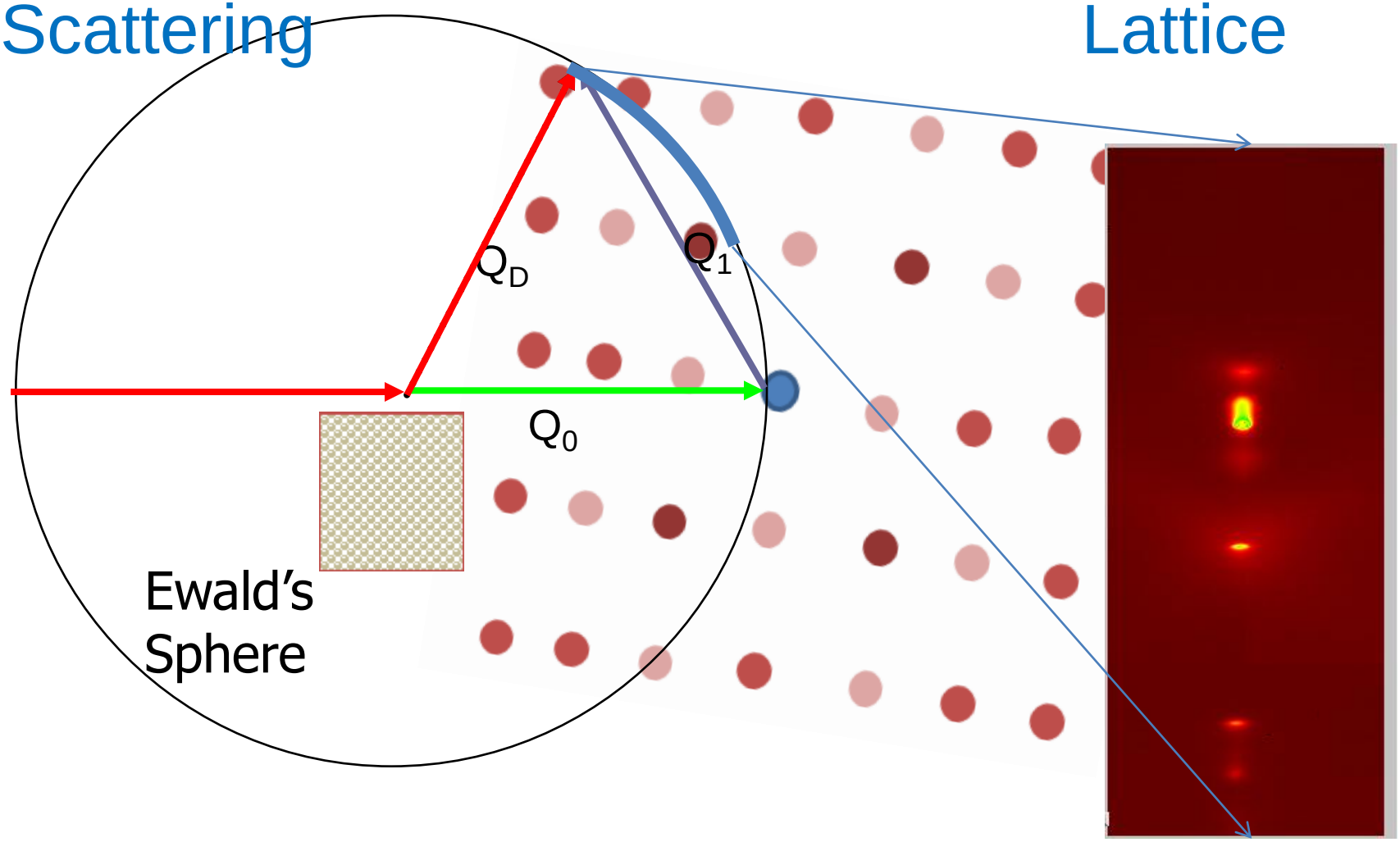
Scattering Pattern and Ewald's Sphere



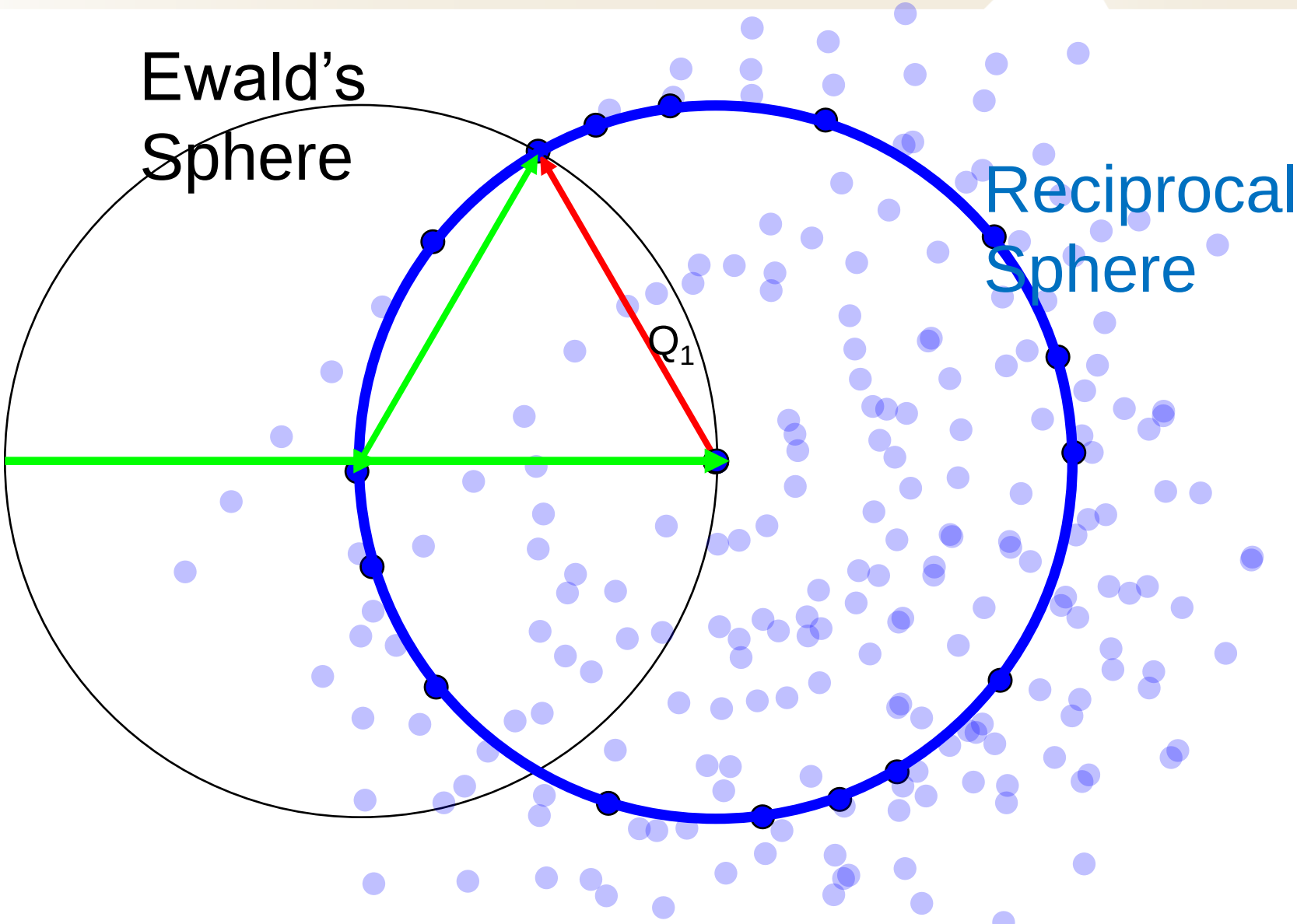
2D detectors and Ewald Sphere

Elastic Scattering

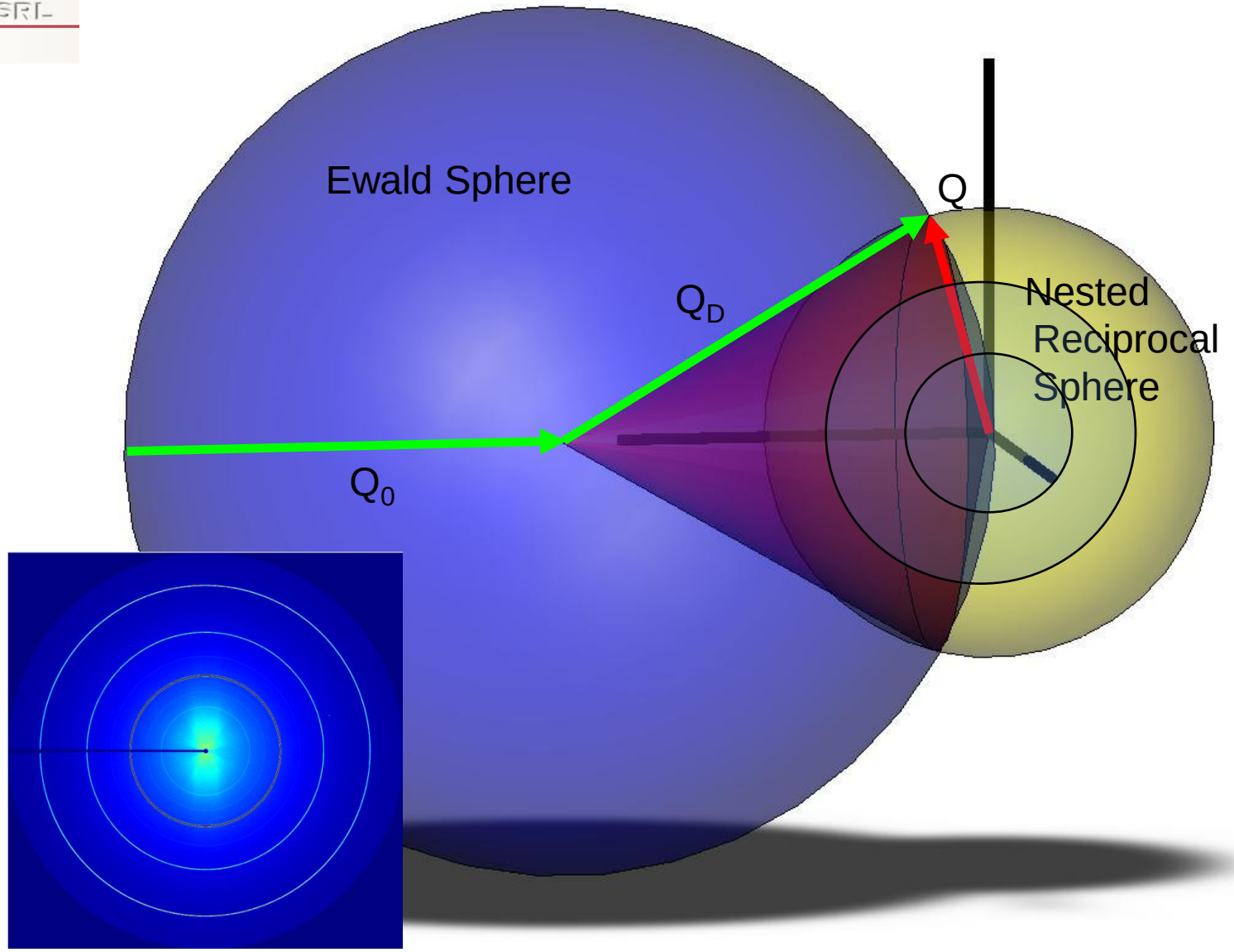
Reciprocal Lattice



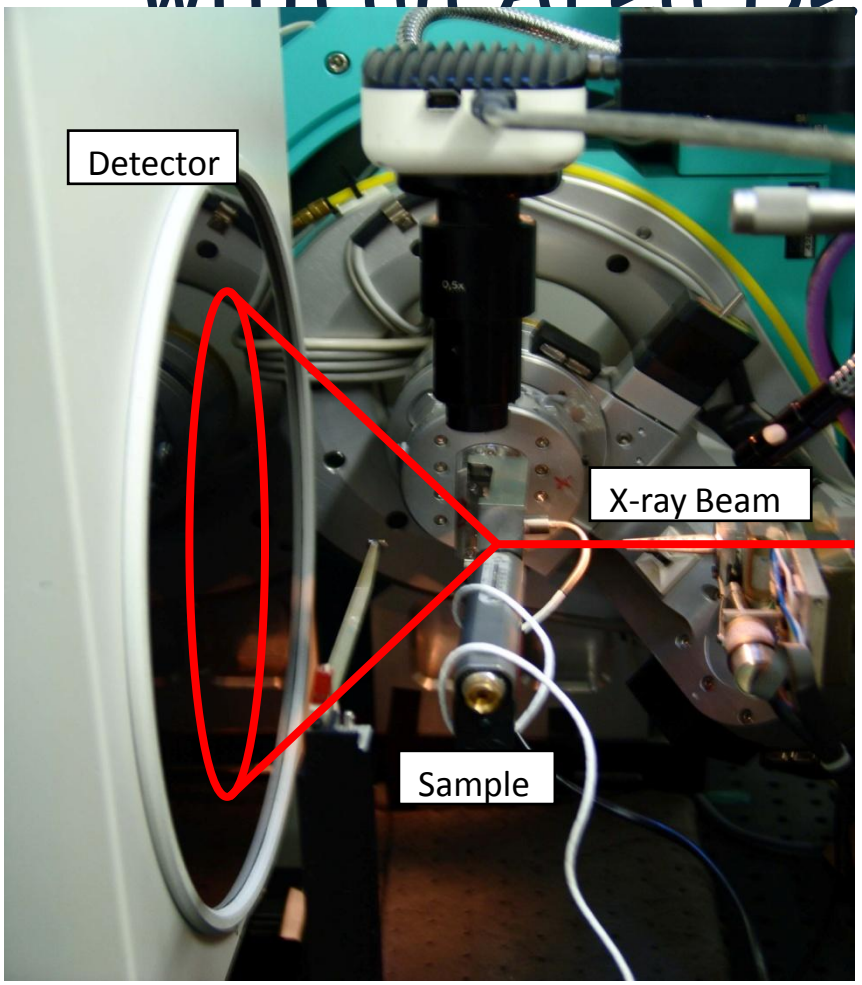
Scattering from Many Crystallites :polycrystal or powder



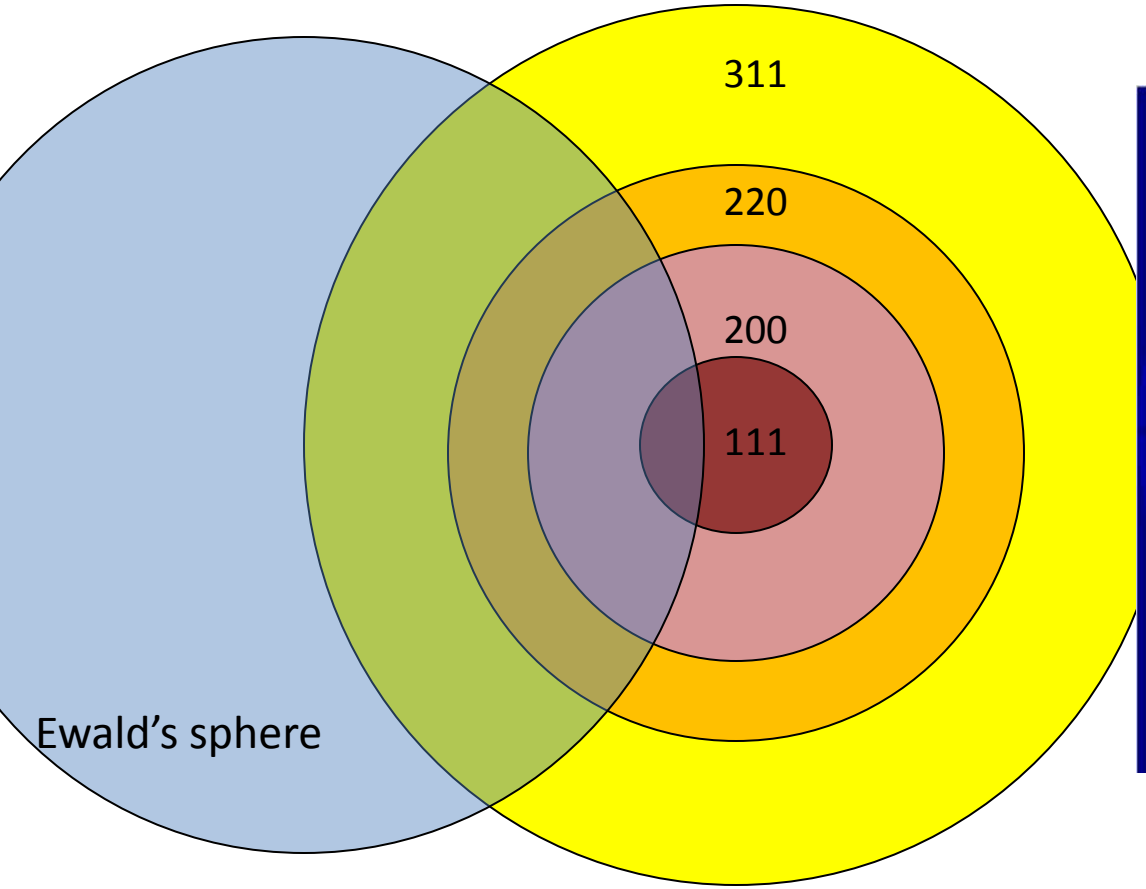
Powder Diffraction Pattern



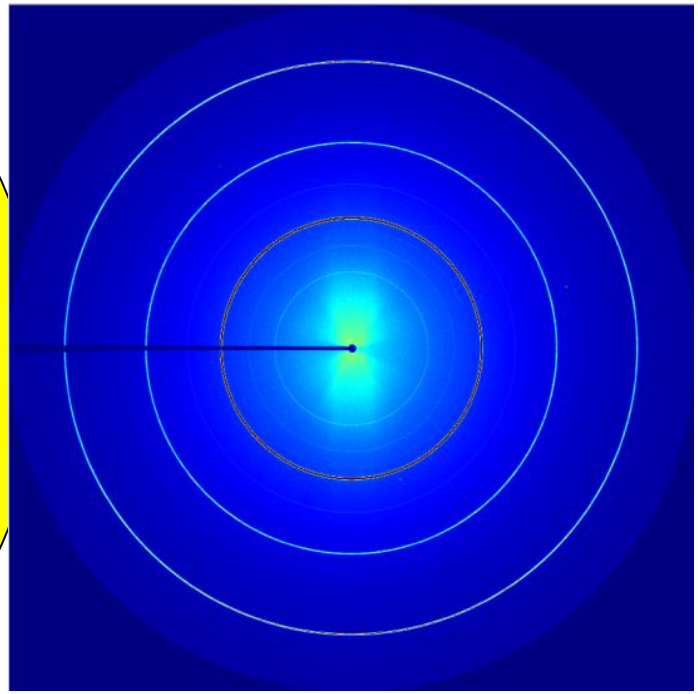
Powder Diffractometer with an Area Detector



Diffraction from Polycrystals

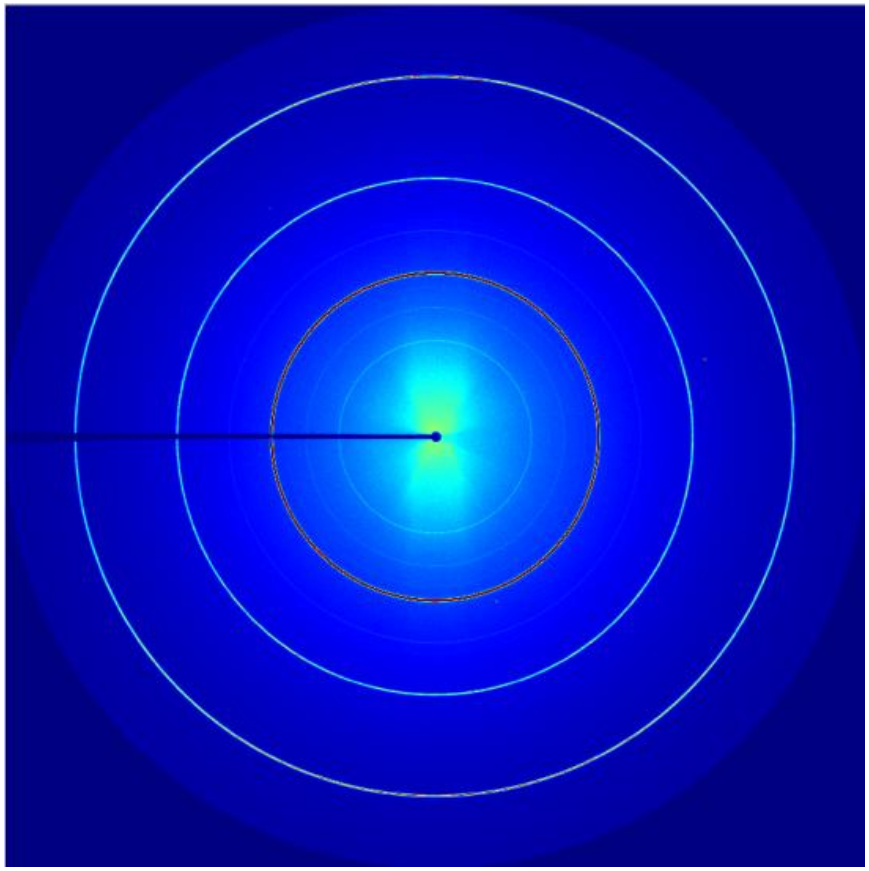


Nested Reciprocal Spheres



Diffraction Pattern

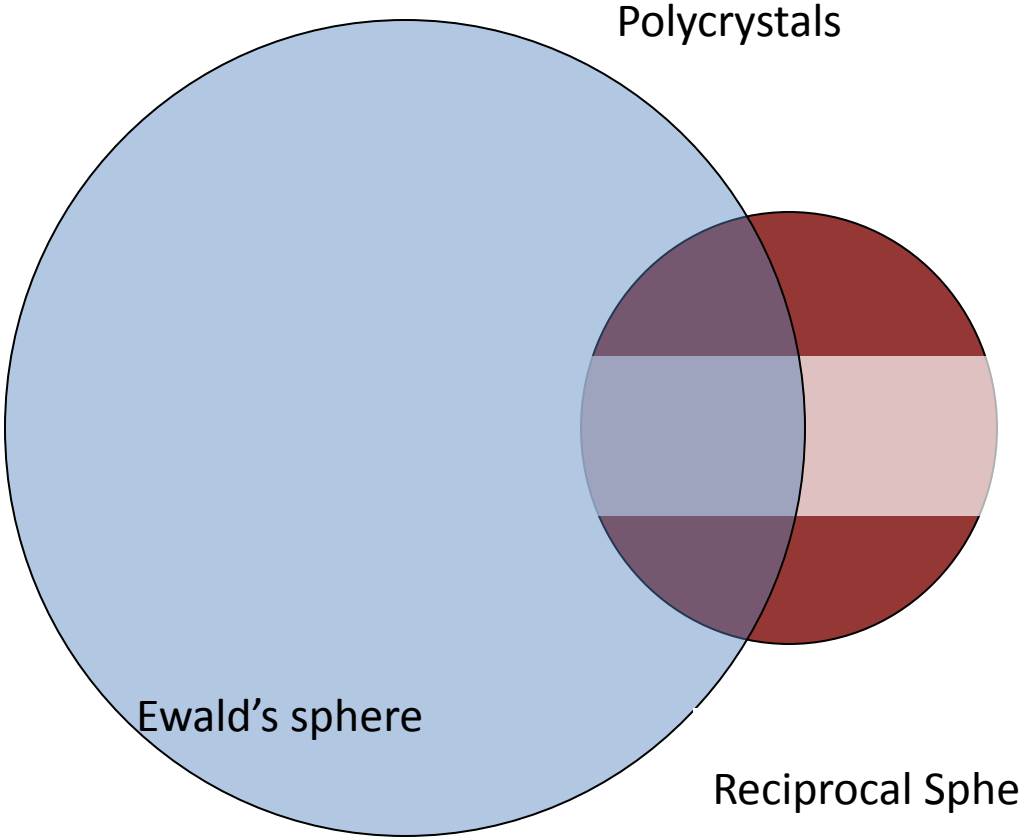
Condition for Polycrystalline/powder Diffraction



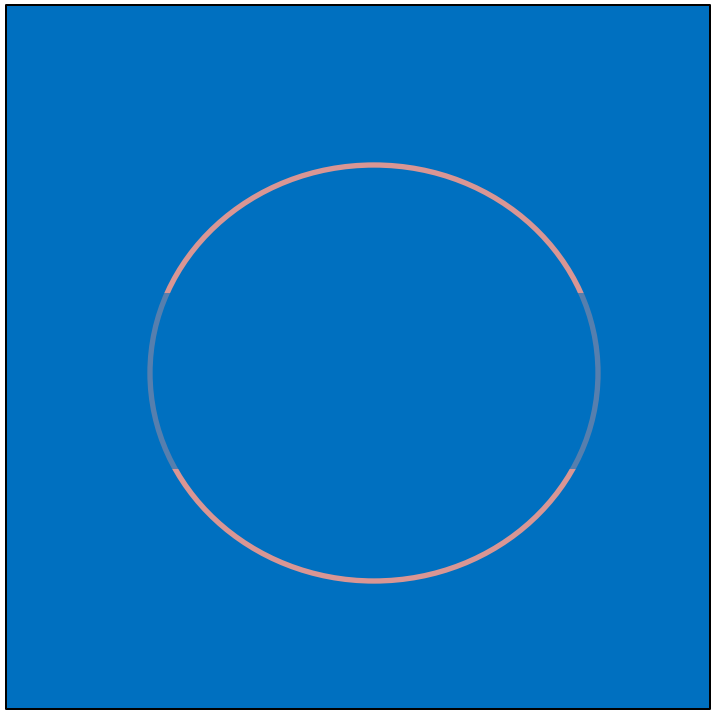
- Just 1 angle (detector)
- If large area detector → 0 angles
- Nothing moves
  - Very useful for fast/time dependent measurements

Texture

Oriented
Polycrystals



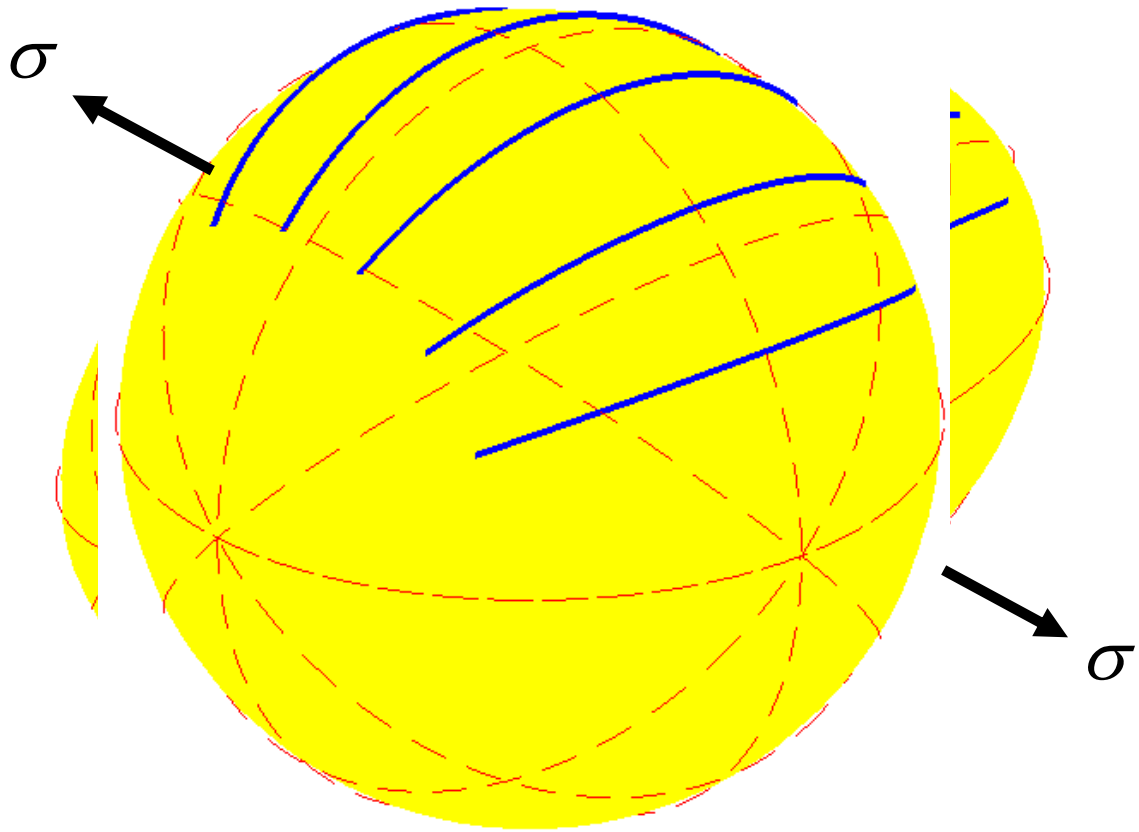
Diffraction pattern



Partial diffraction ring

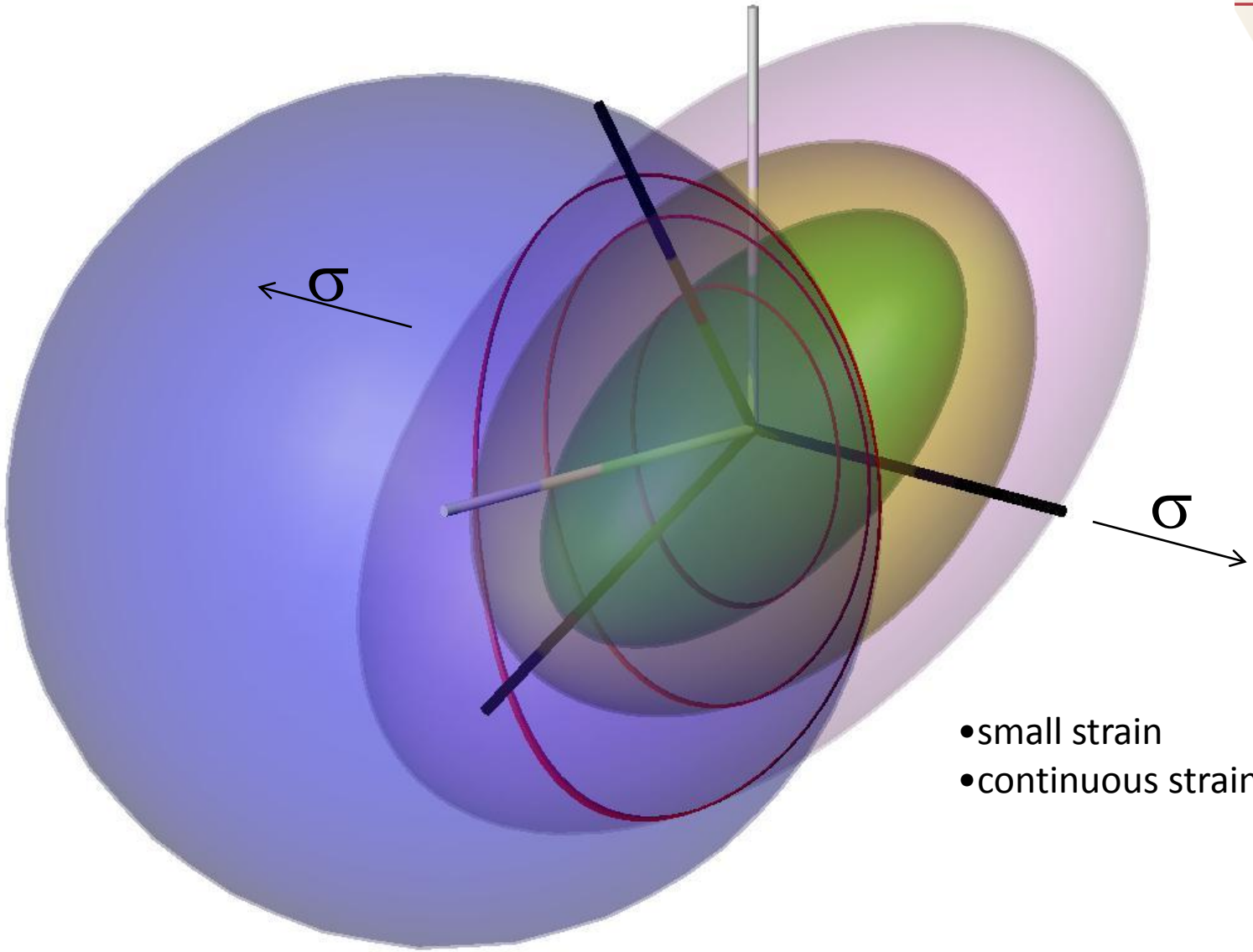
Deformation of Reciprocal sphere

$$u_i = \epsilon_{ij} k_{0_j}$$



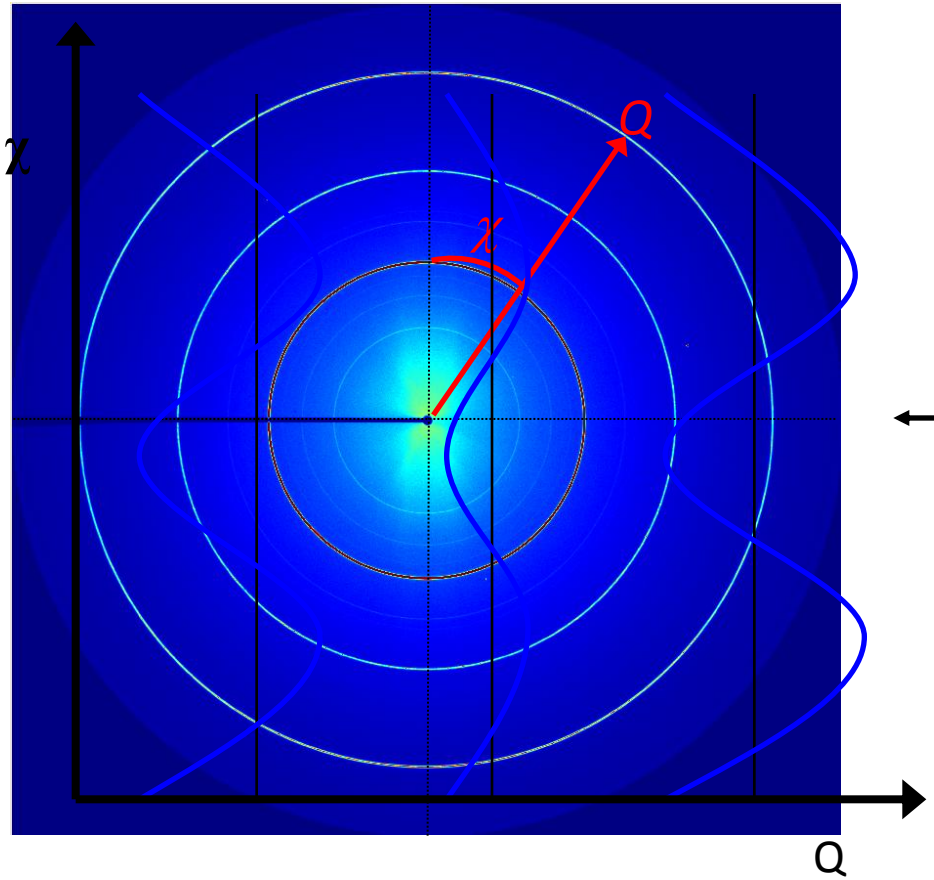
Strain Ellipsoid

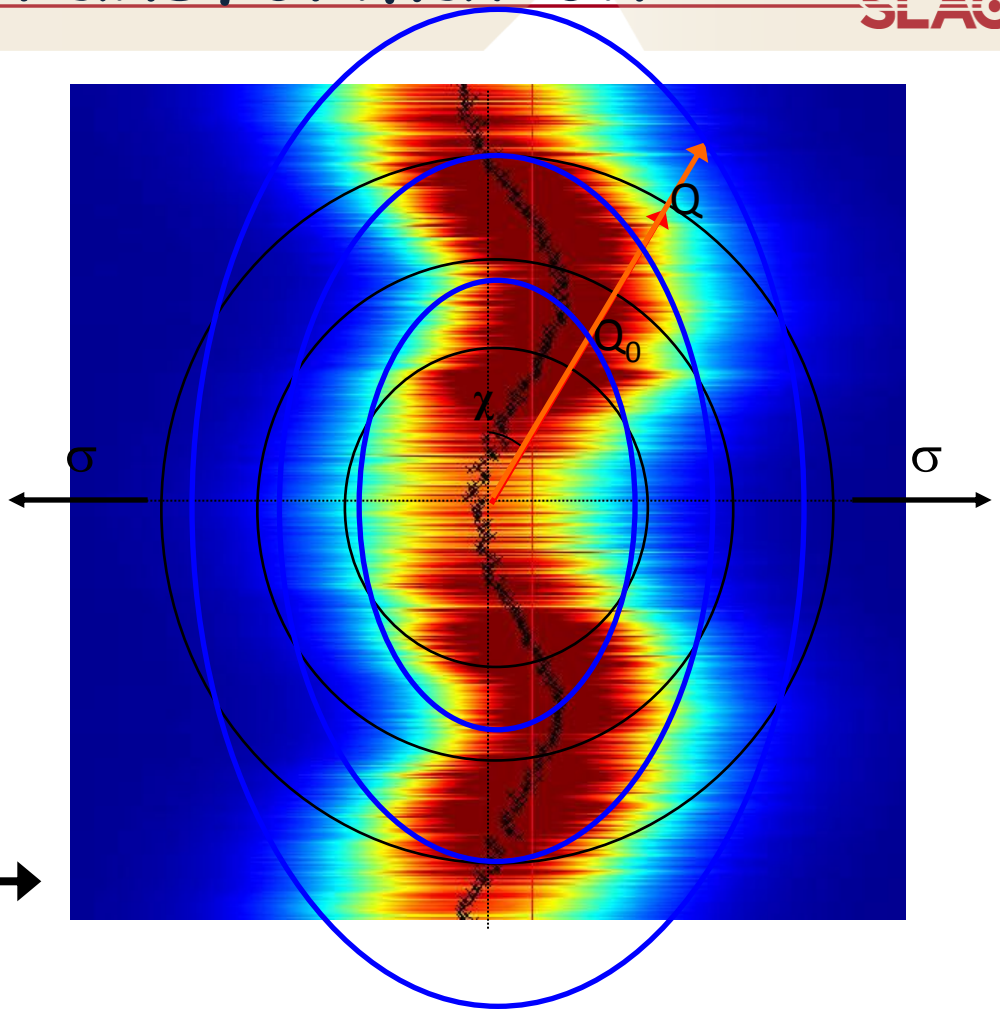
Strain Ellipsoid



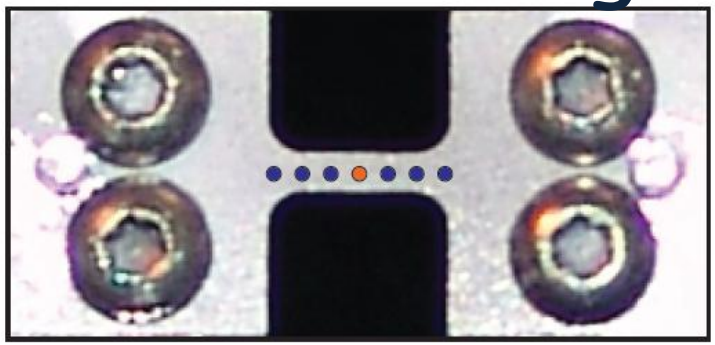
- small strain
- continuous strain

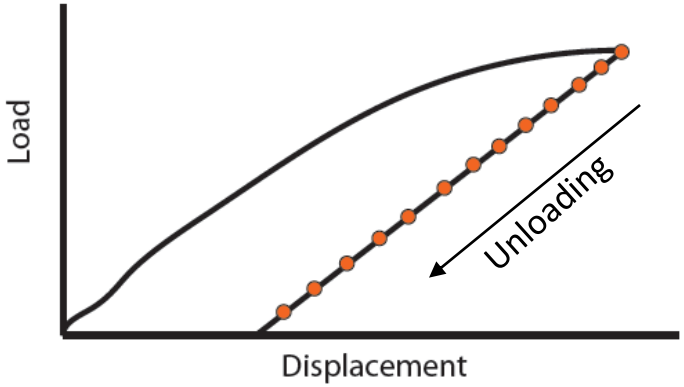
Coordinate transformation



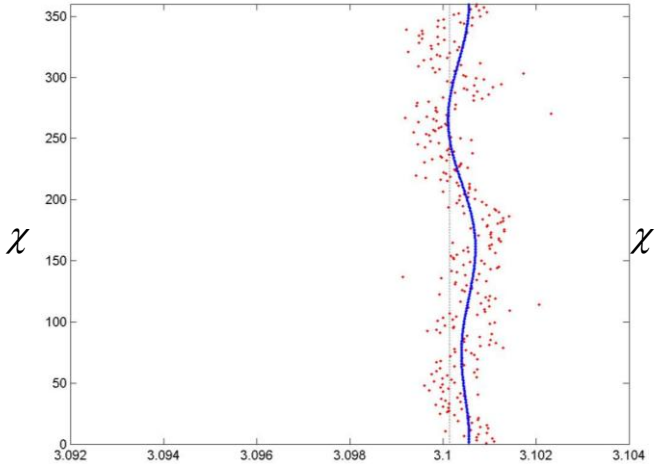


Measuring Full Strain Tensor

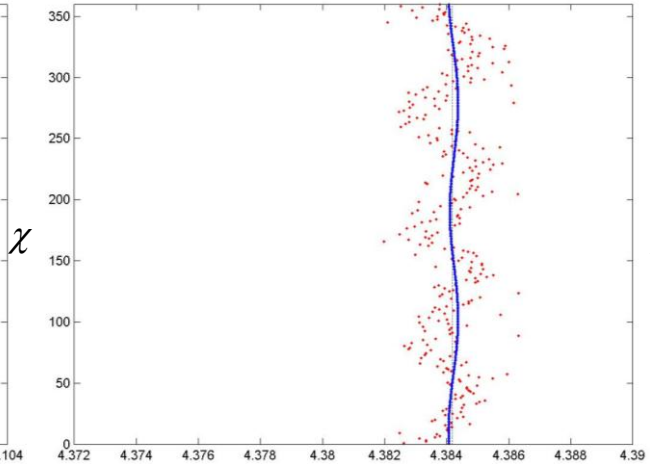




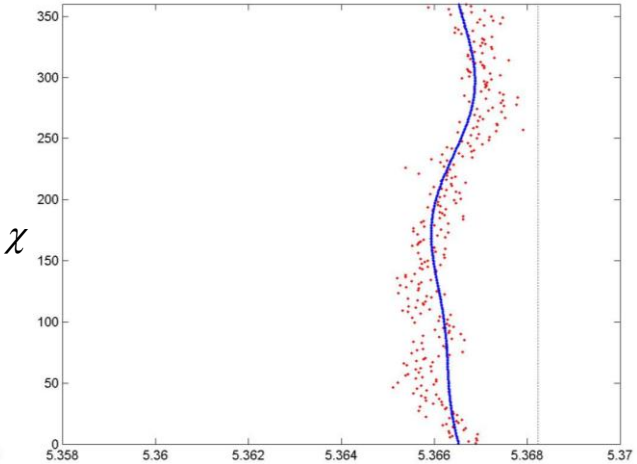
110



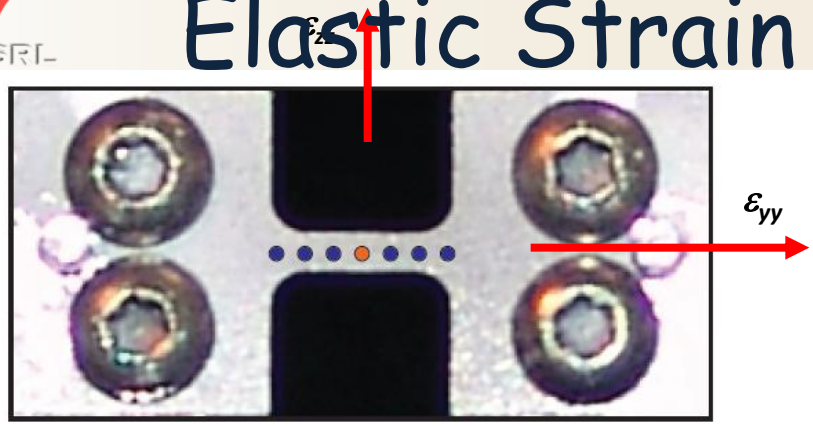
200

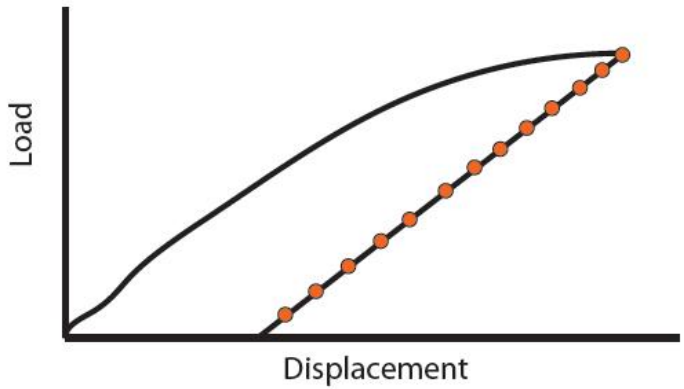


211

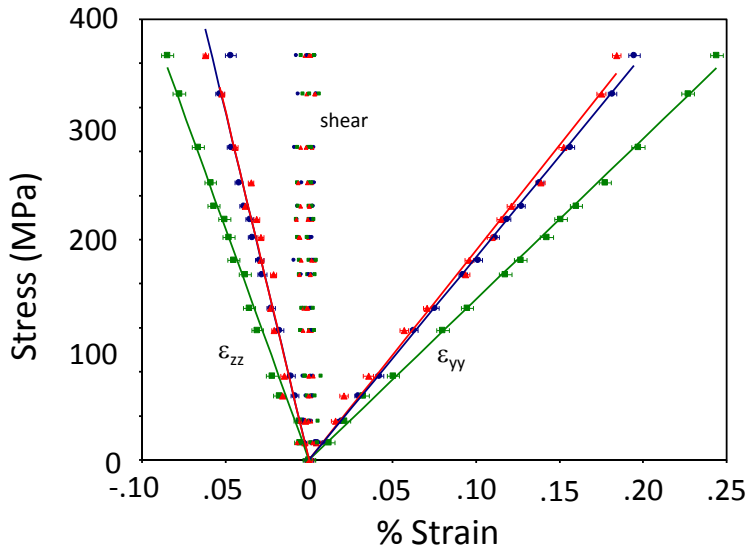


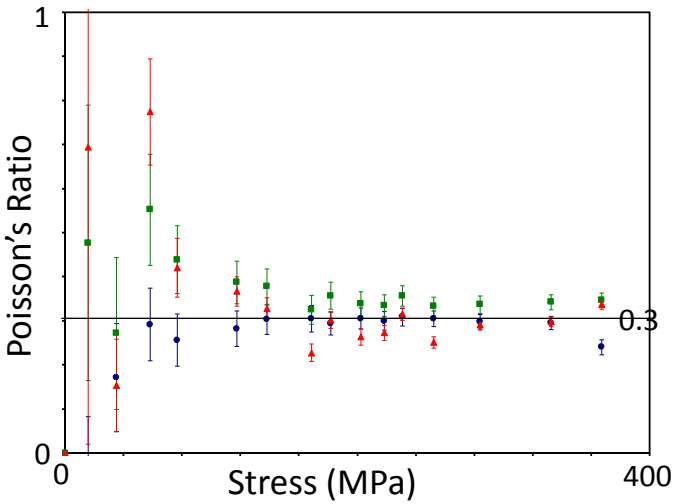
Elastic Strain Tensors for Fe





110 E_m = 211 GPa 200 E_m = 167 GPa 211 E_m = 218 GPa

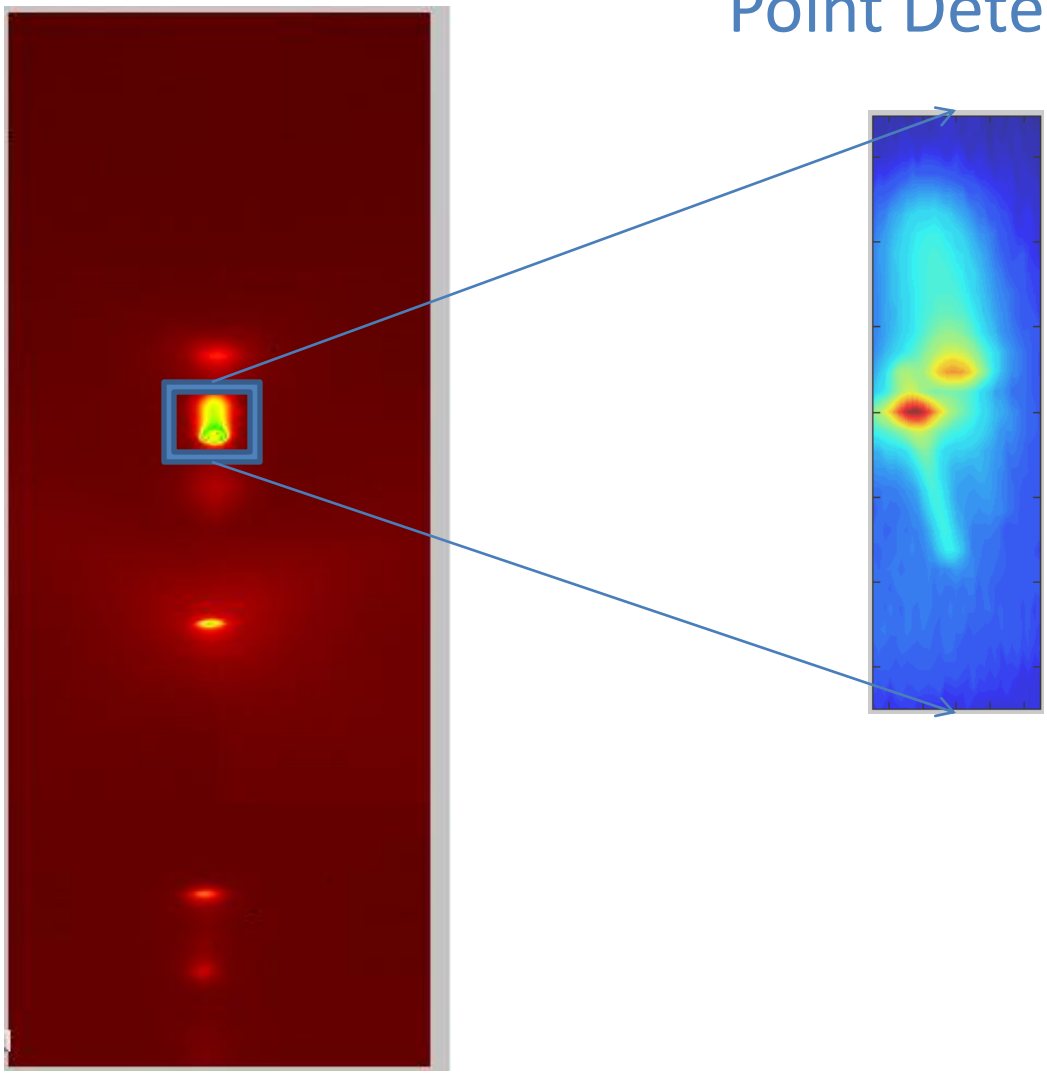




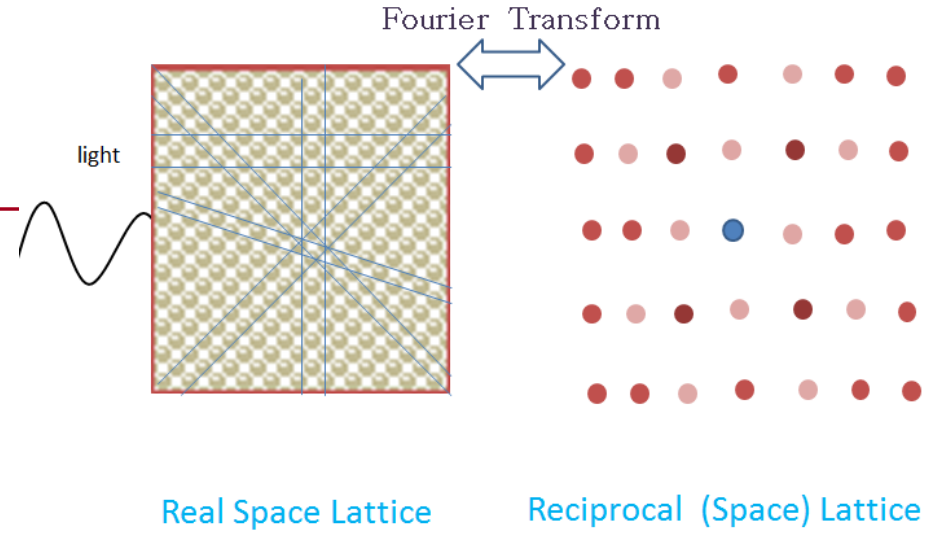
Resolution

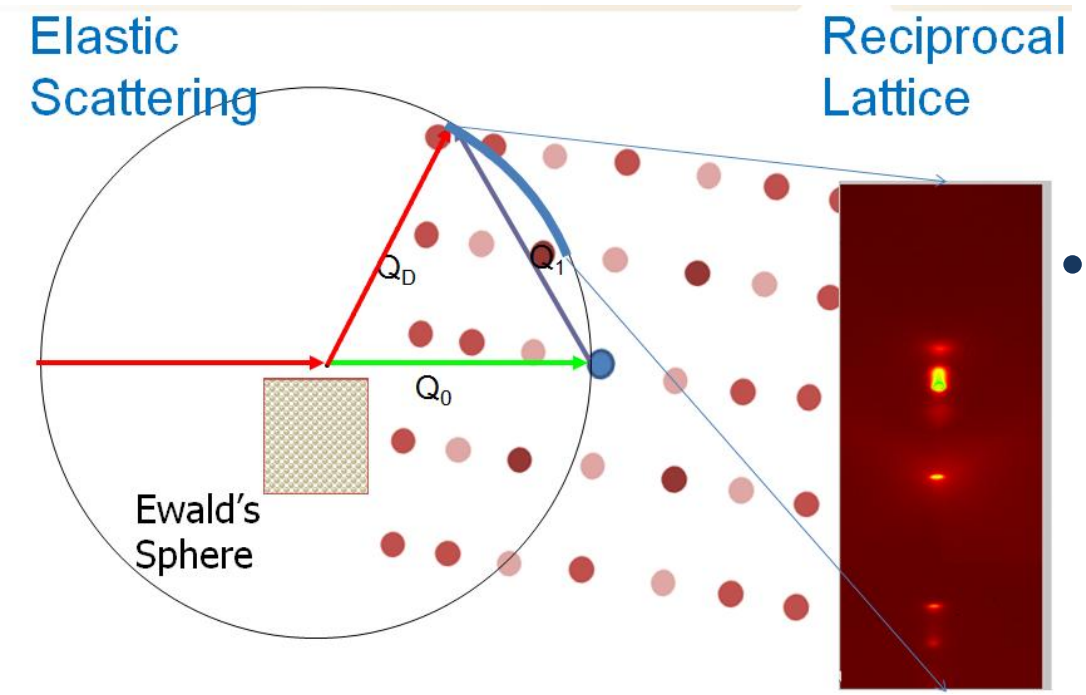
Area Detector

Point Detector

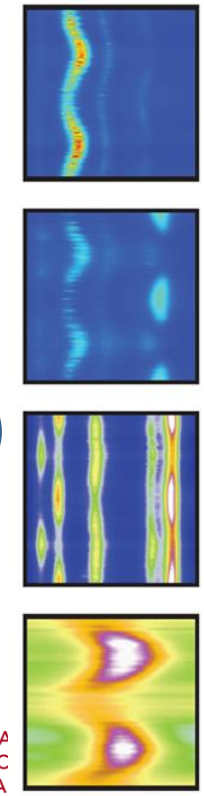


Questions?





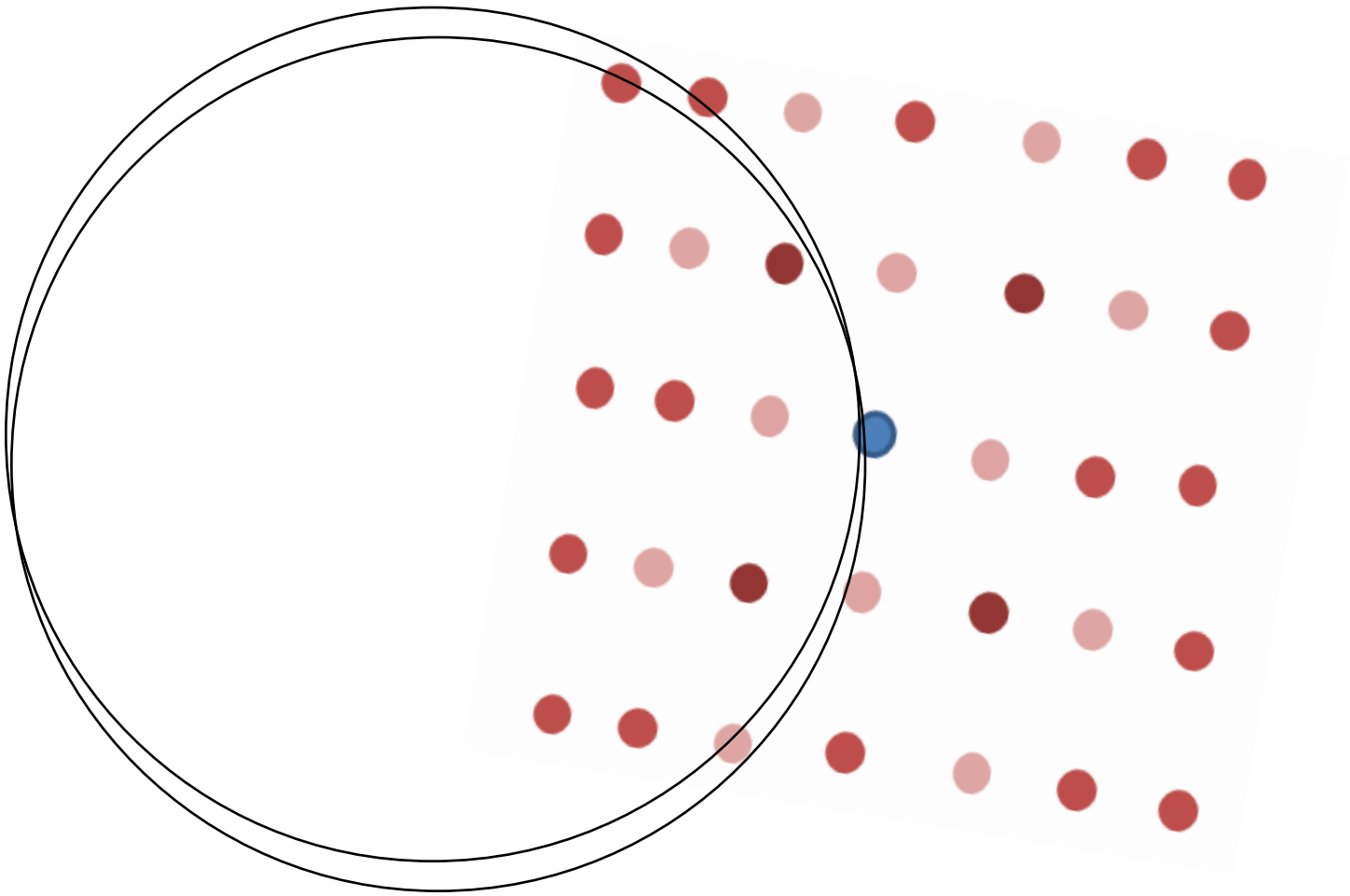
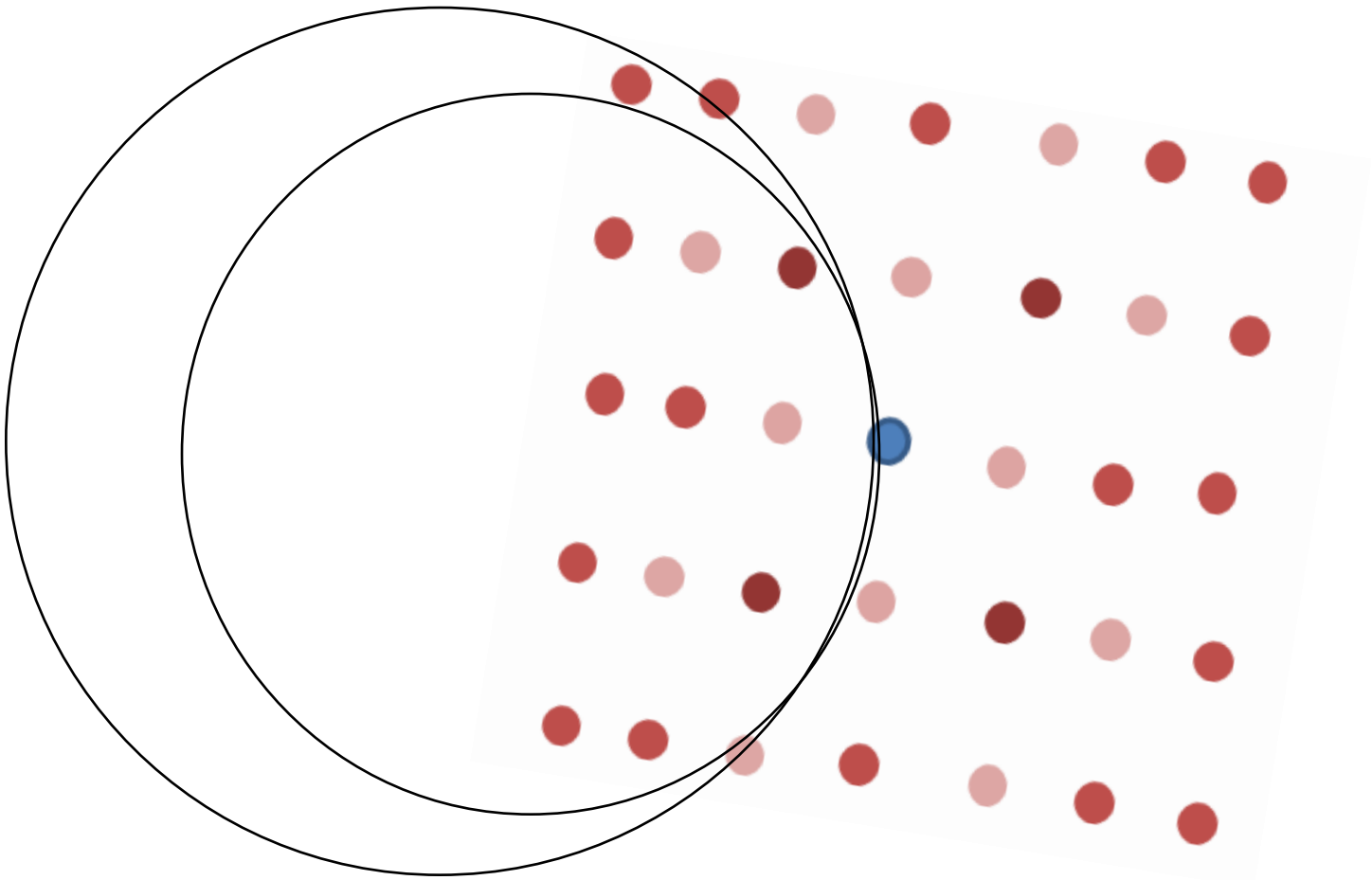
- Think in Q space
  - (yardstick of reciprocal space)
  - $Q = 4\pi \sin(\theta) / \lambda$



U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Effect of Beam Divergence



Effect of Energy Width