Thinking in Reciprocal Space

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SSRL

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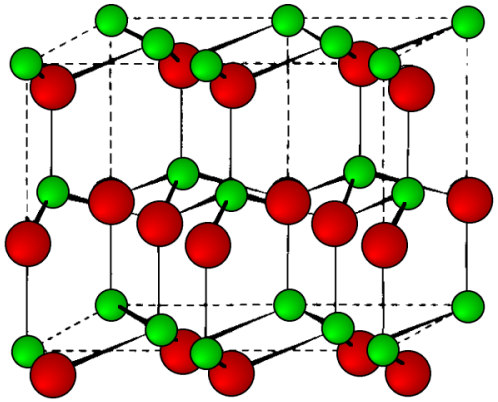
Outline

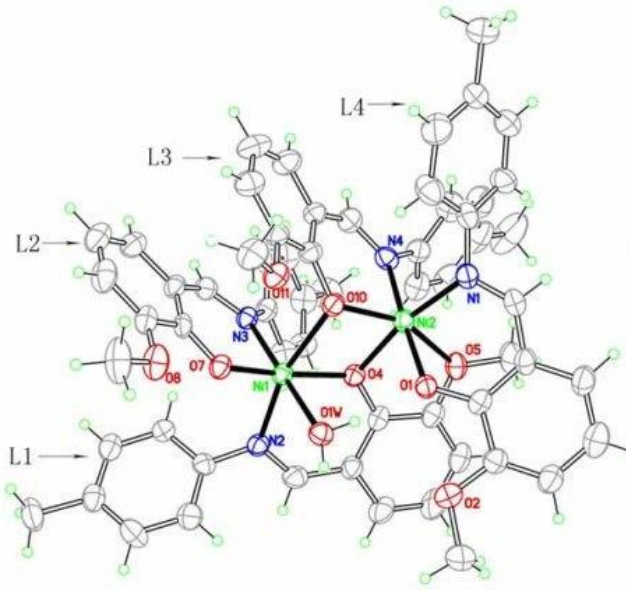
- Introduce Reciprocal Space

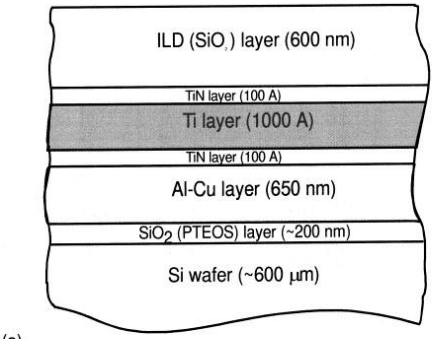
- Reciprocal Space maybe at first appear strange
  - Examples → thinking in reciprocal space makes intepretting scattering experiments easier.

Why X-ray Scattering?

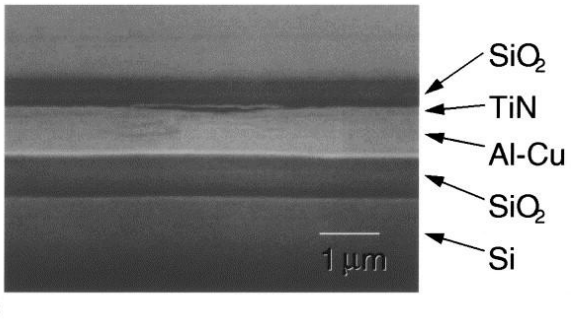
- Structure of Materials
  - 10s of nm to A







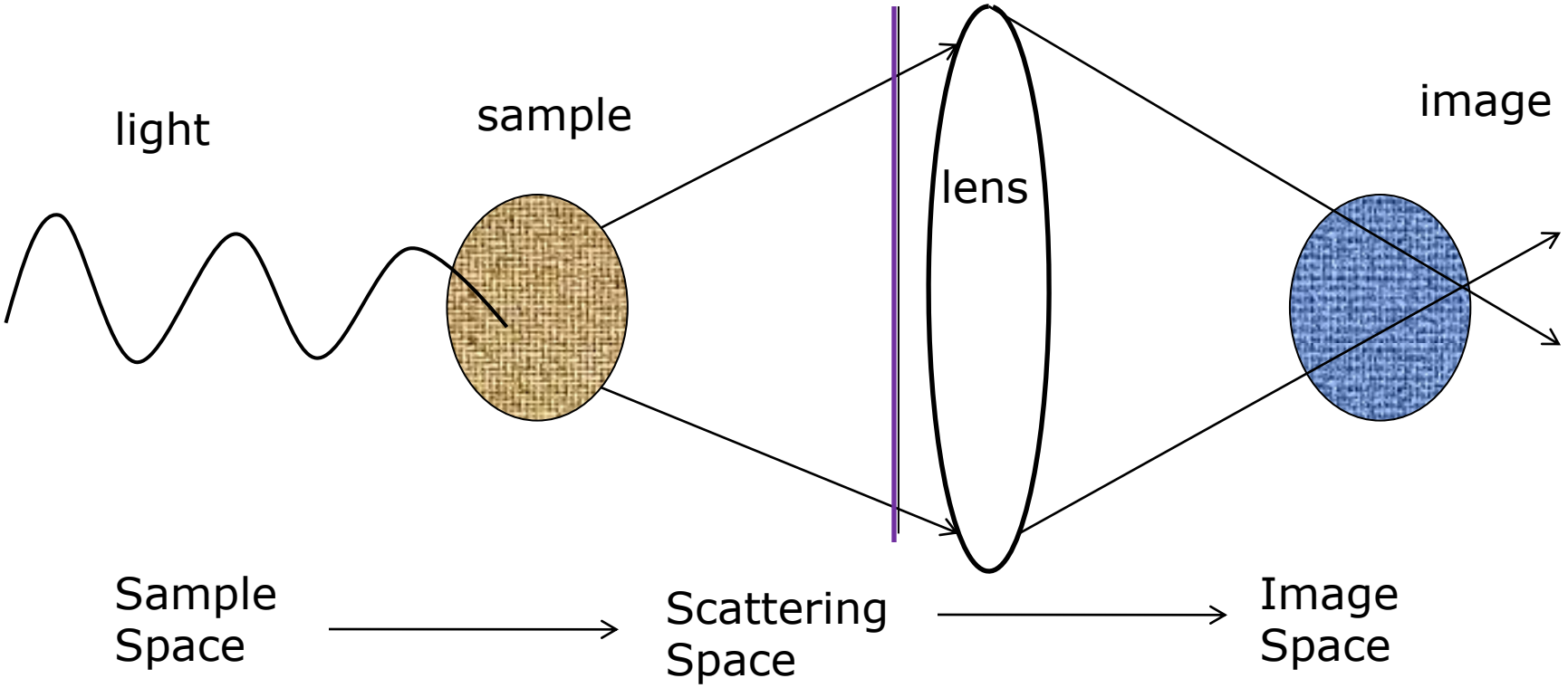
(a)



(b)

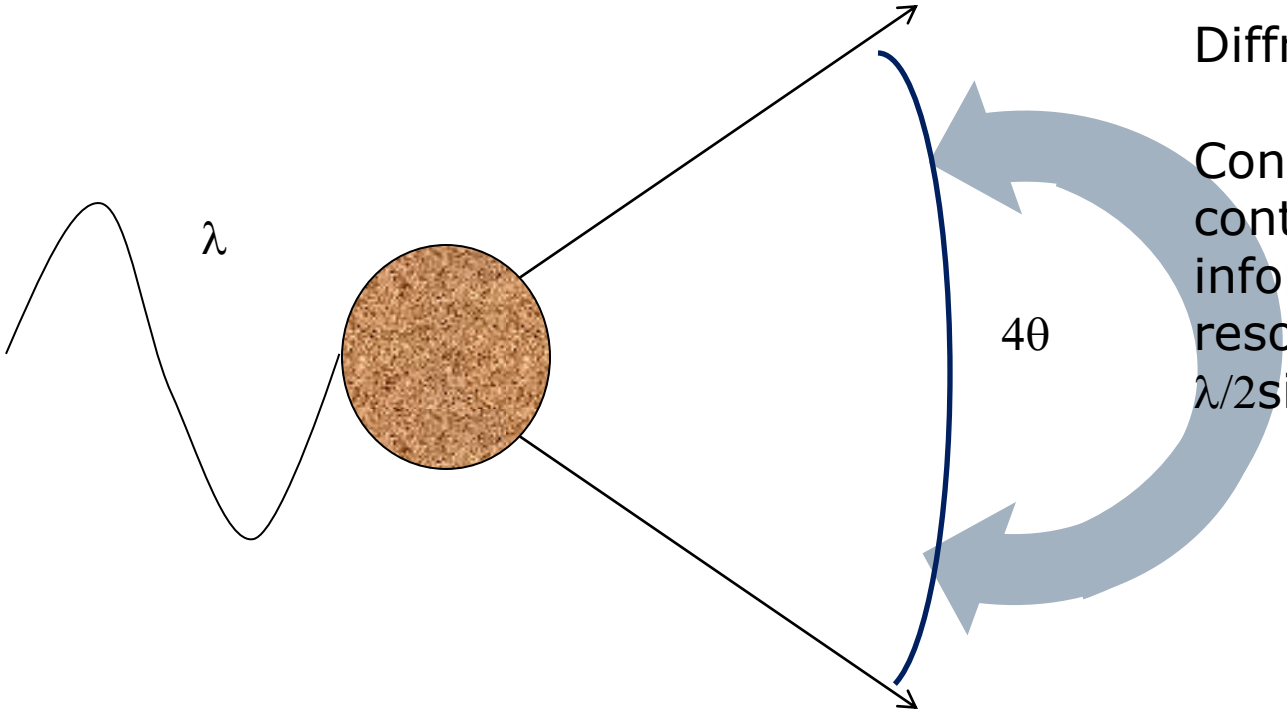
Scattering Physics

X-ray lens with resolution better than ~10nm don't exist



X-ray Scattering/diffraction is about probing the structure without a lens

Sample to Scattering Space



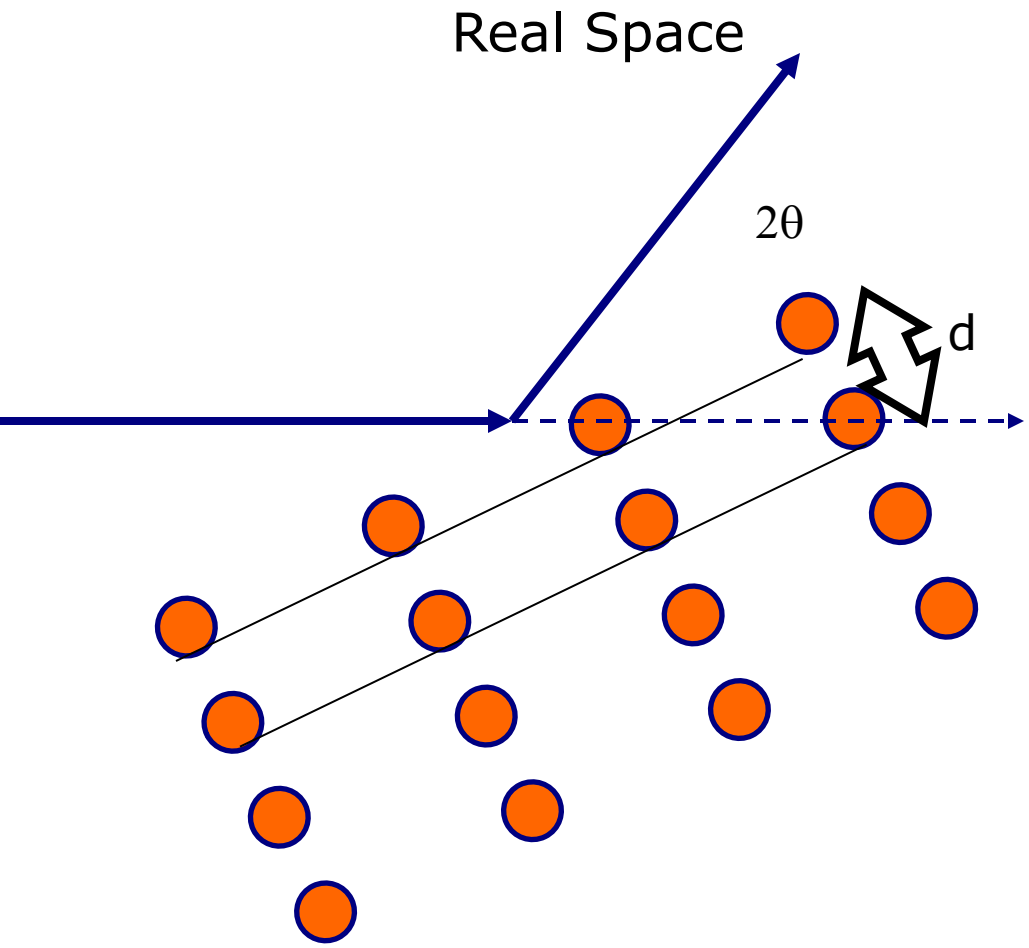
Diffraction Pattern:

Contains all the contrast relevant information at the resolution of $\lambda/2\sin(\theta)$

Transformation of distance into angle

Fourier Transform: sample space → scattering space

Scattering Physics: Bragg's Law



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

$1/2d = \sin(\theta)/\lambda$

1. Distance ←→ Angle

   "Reciprocal" relation

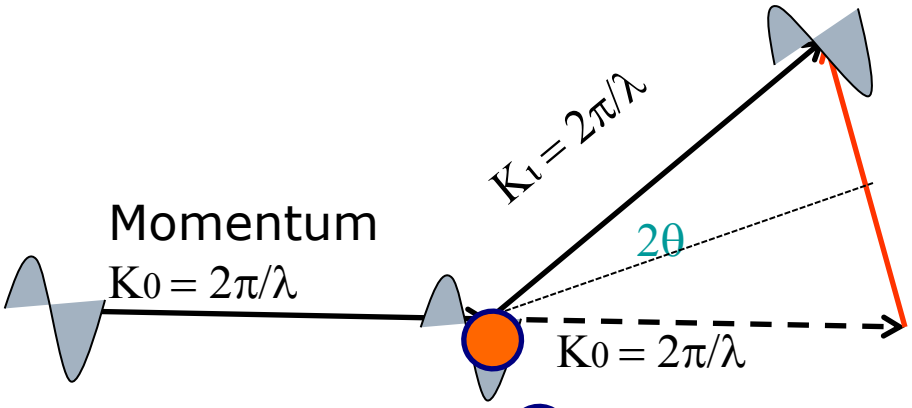
2. Fundamental unit is not θ but $\sin(\theta)/\lambda$

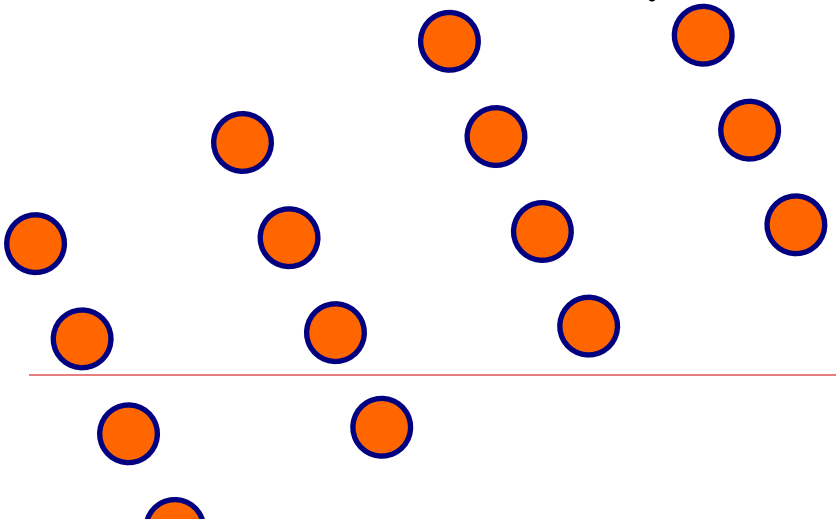
Fundamental Units for scattering

- $s = \sin(\theta)/\lambda$
- $Q = 4\pi \sin(\theta)/\lambda$
- Think in Q
- Or provide both θ and λ
  - λ= hc/E – synchrotron units are E

Scattering Physics

Elastic
Scattering





Momentum change

$\Delta K = 2\sin(\theta) * 2\pi/\lambda$

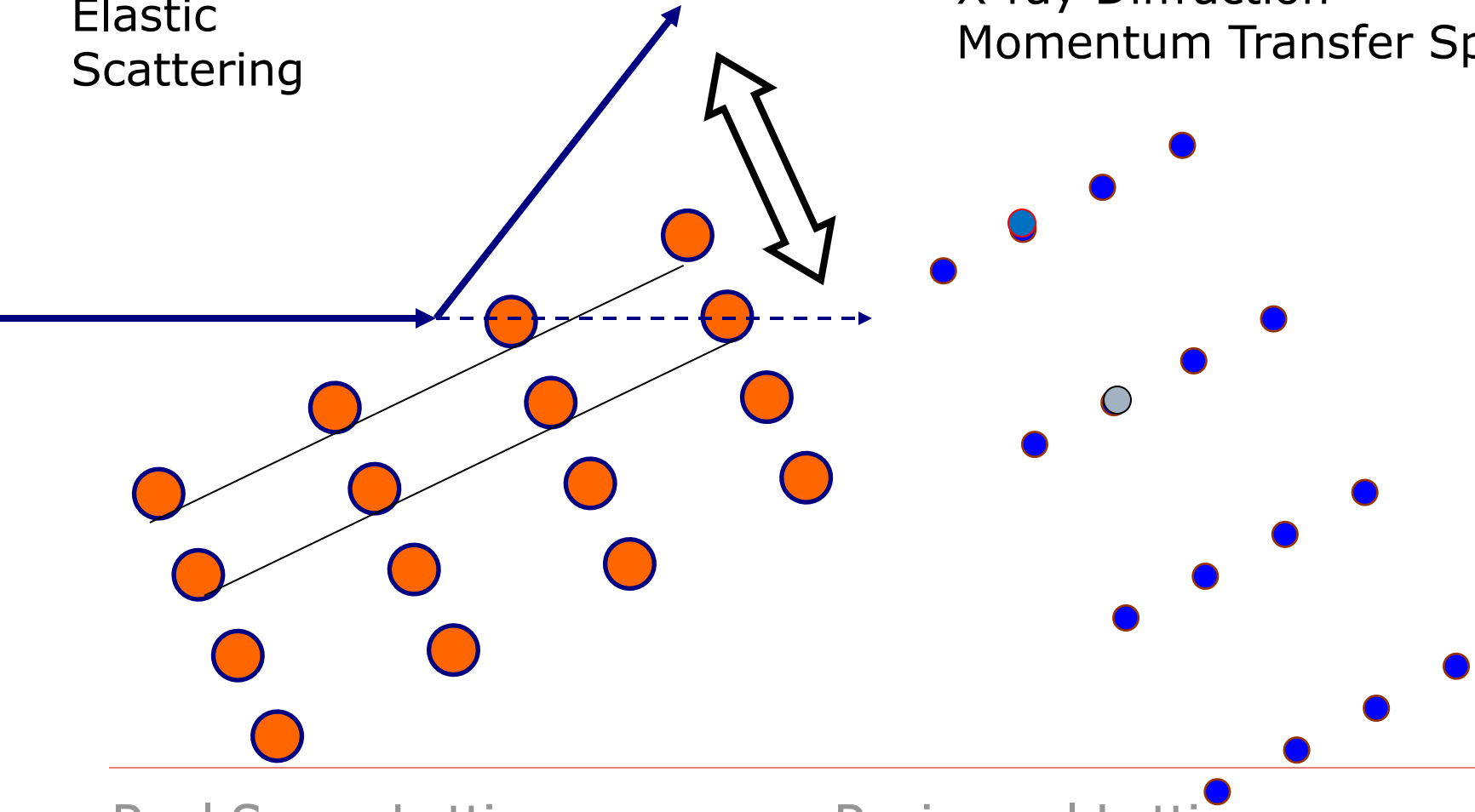
$\Delta K = Q = 4\pi \sin(\theta)/\lambda$

Reciprocal Space

Ordered Lattice can only provide discrete momentum kicks: Bloch

Elastic Scattering

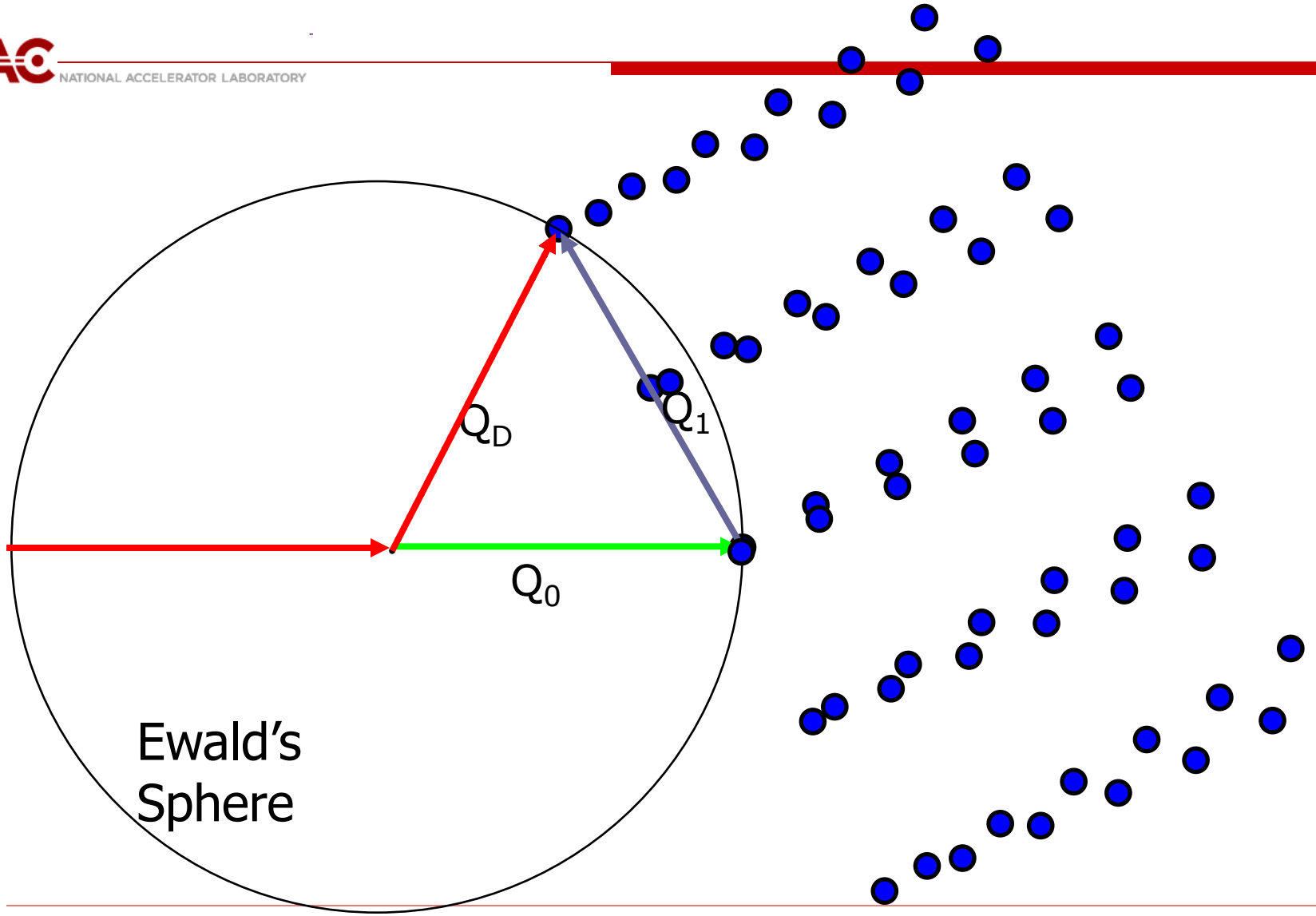
X-ray Diffraction Momentum Transfer Space



Real Space Lattice

Reciprocal Lattice

Graphical Solution: Single crystal

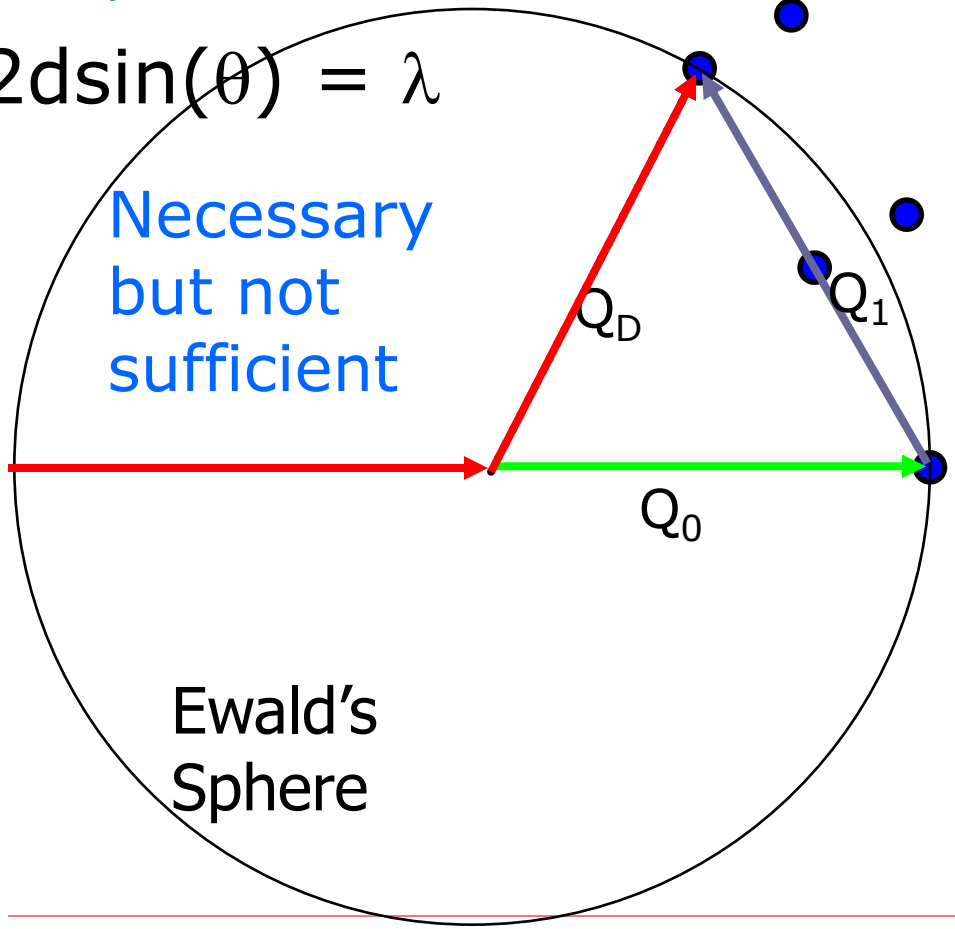


Conditions for Single Crystal Diffraction

Bragg's law provides condition for only the detector

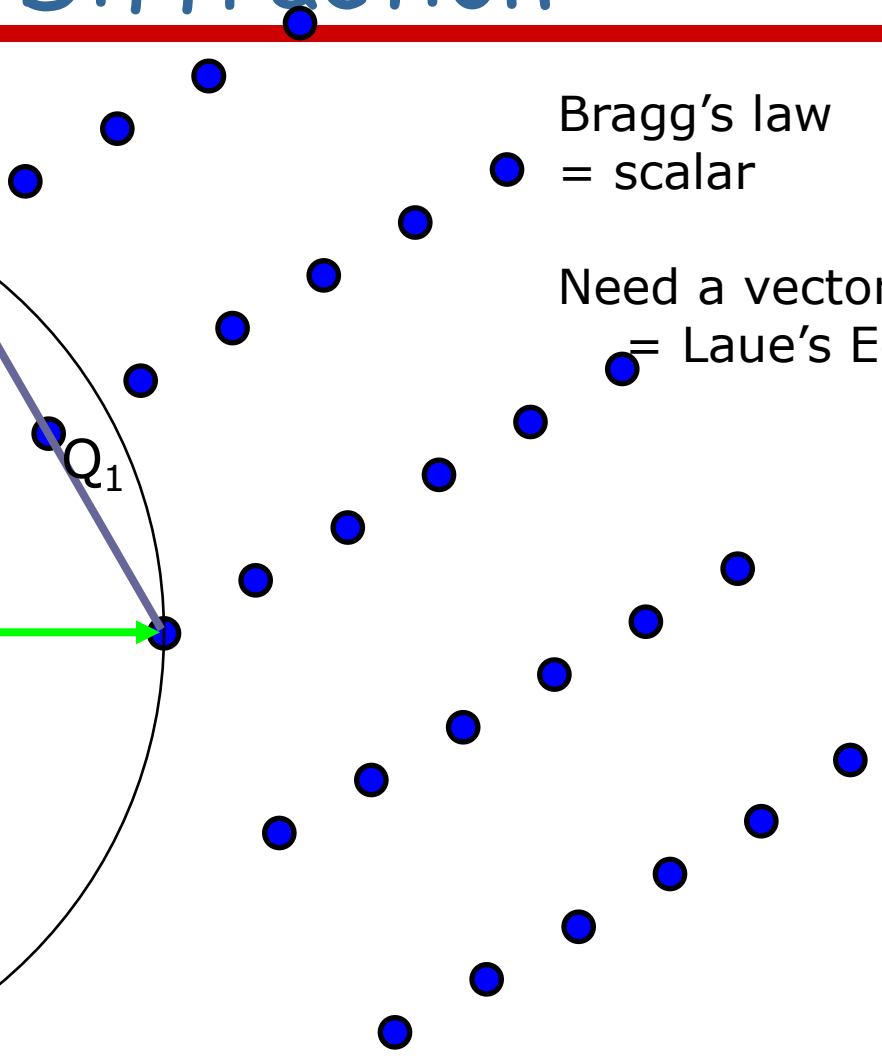
$2d\sin(\theta) = \lambda$

Necessary but not sufficient



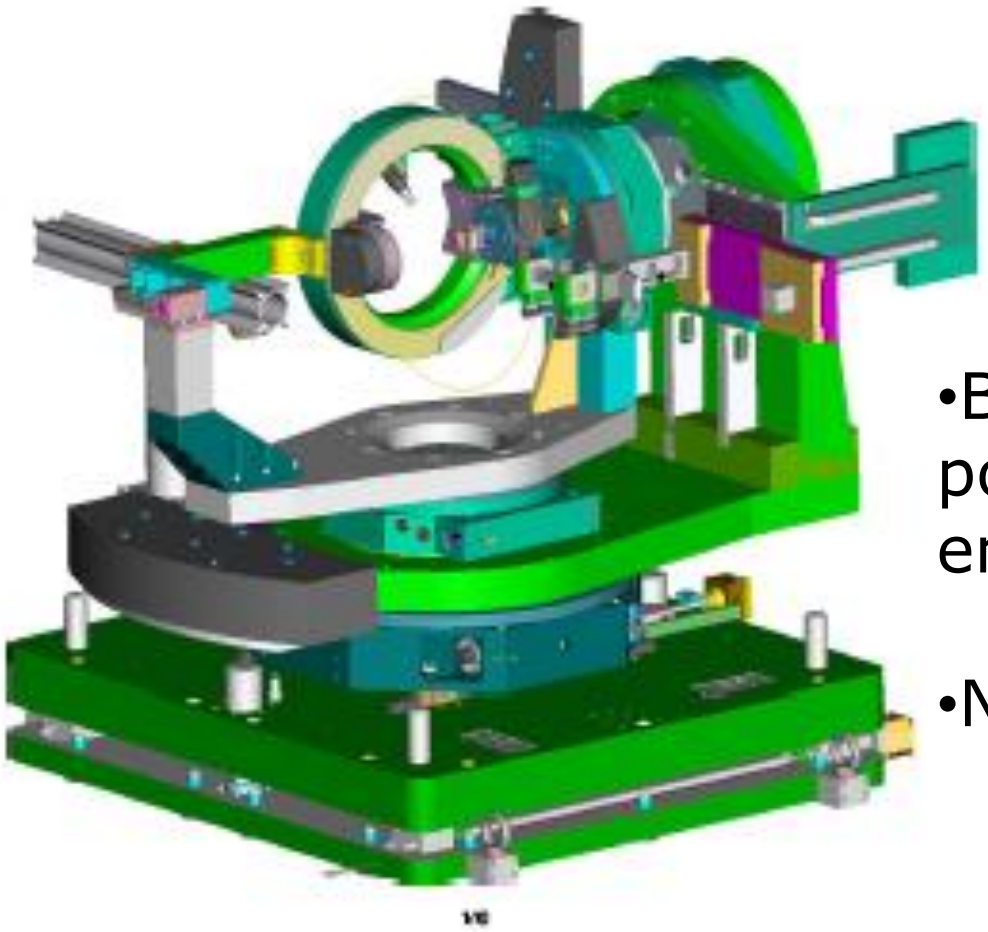
Bragg's law = scalar

Need a vector law = Laue's Eq



Detector AND the crystal at desired location/angles.

Multi-circle diffractometer

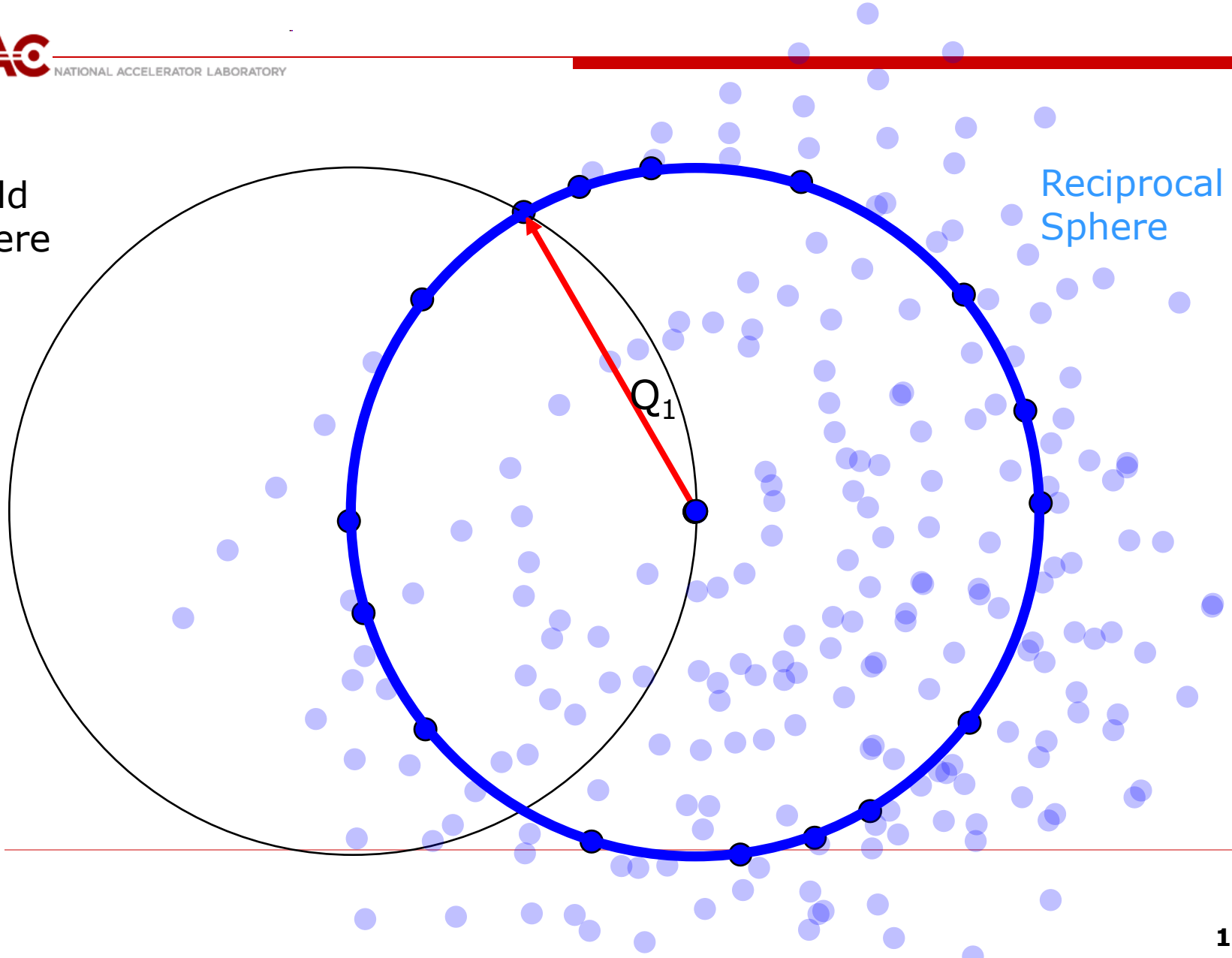


- Need at least
  - 2 angles for the sample
  - 1 for the detector

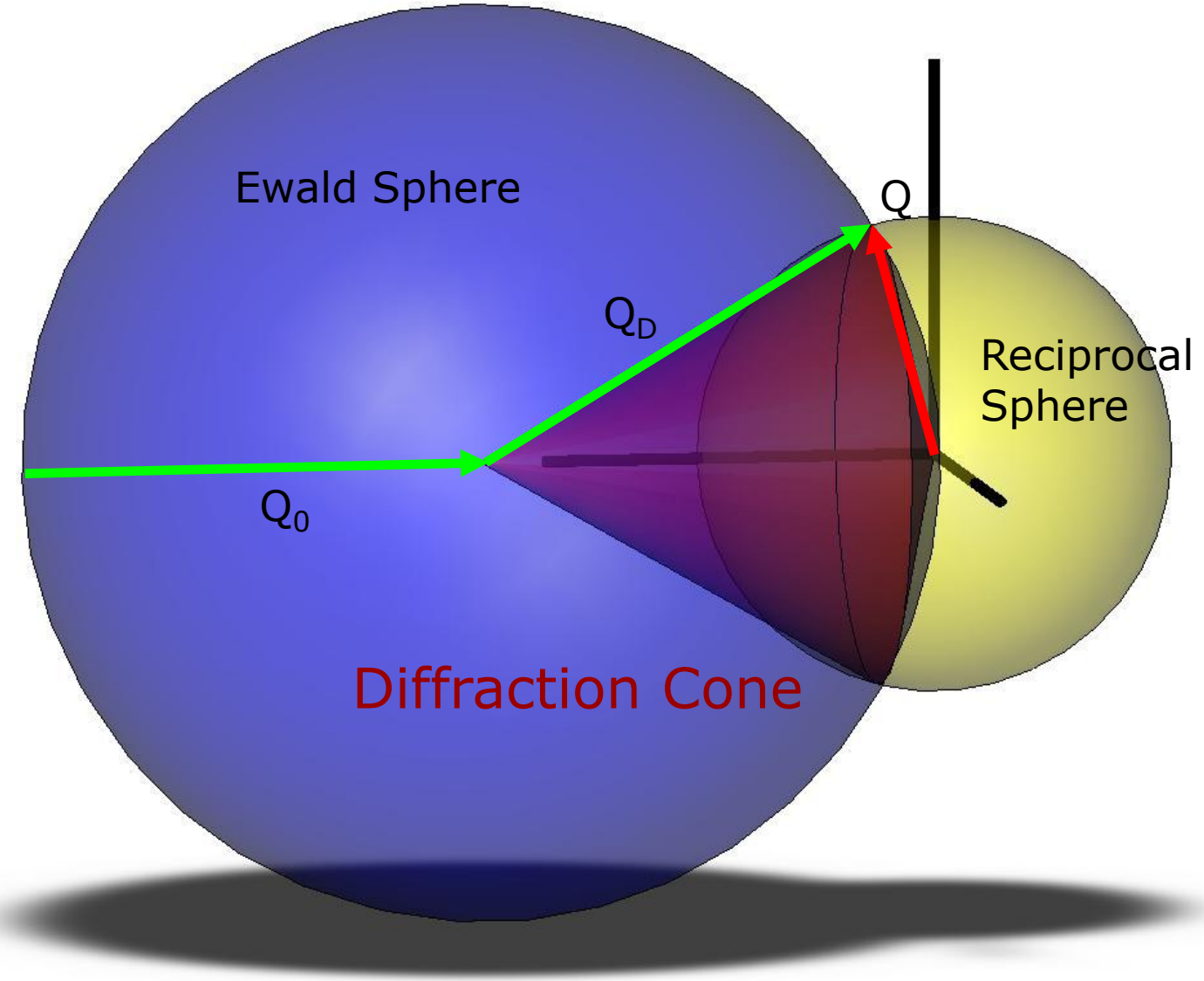
- But often more for ease, polarization control, environmental chambers

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

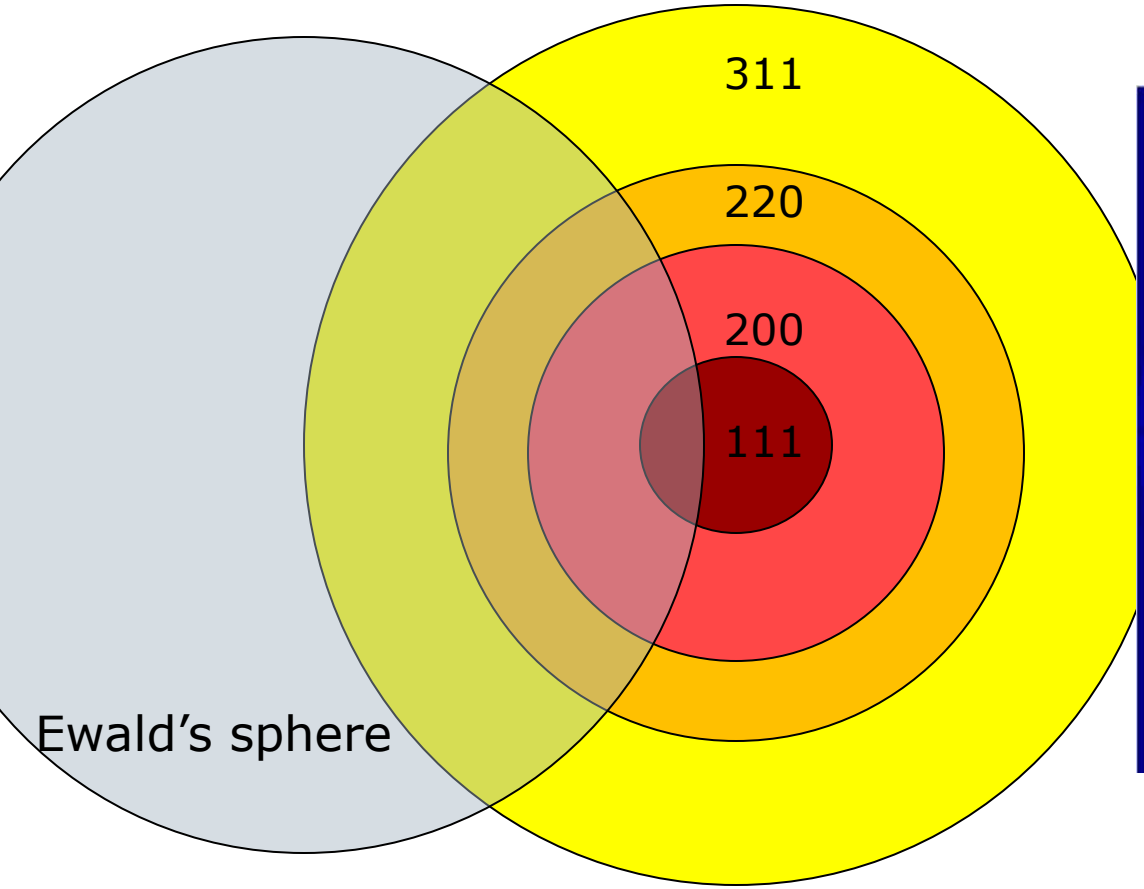
Diffraction from Polycrystals



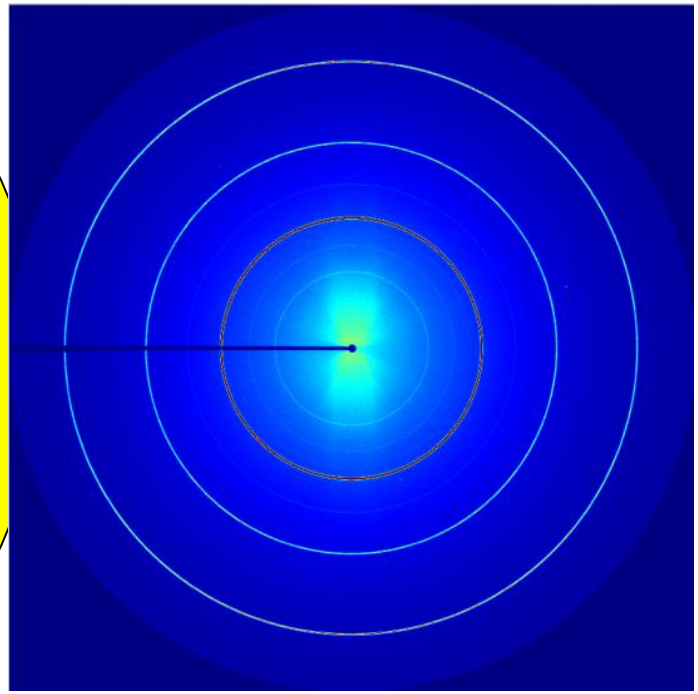
Diffraction from Polycrystals



Diffraction from Polycrystals

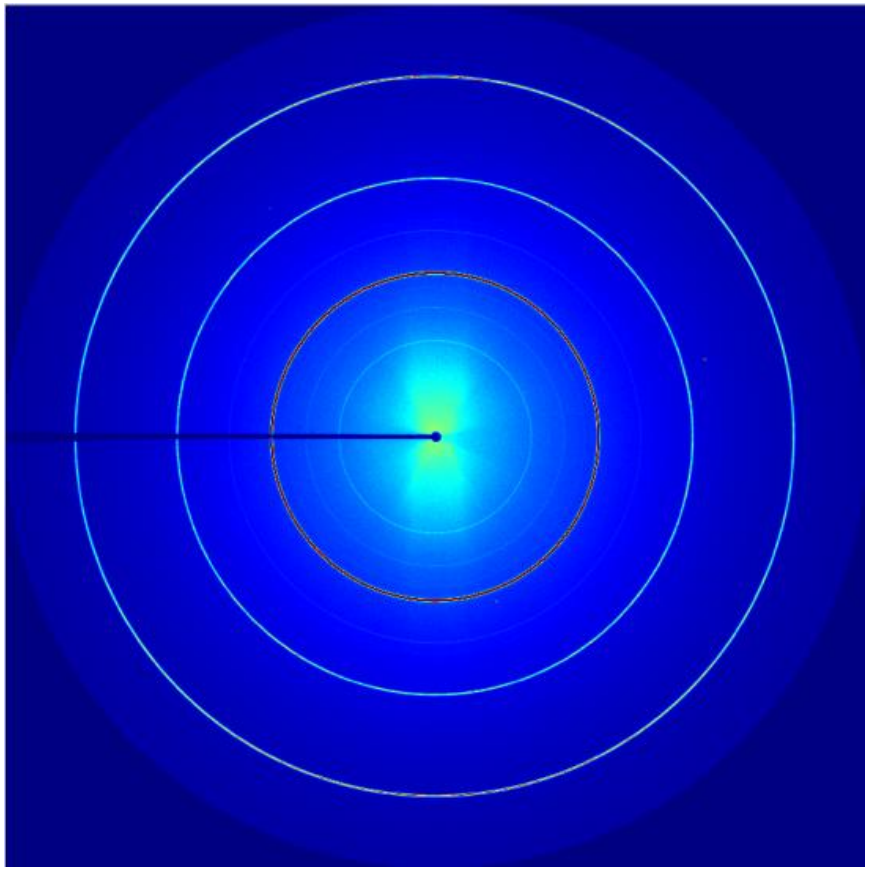


Nested Reciprocal Spheres



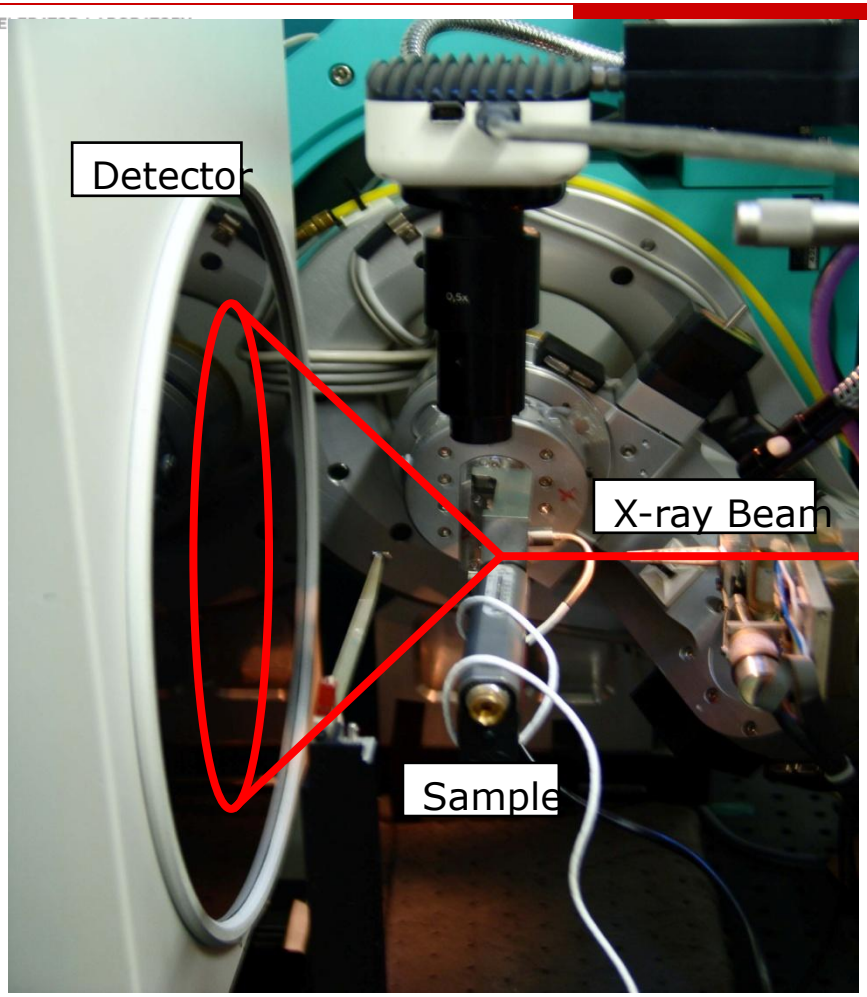
Diffraction Pattern

Condition for Polycrystalline/powder Diffraction

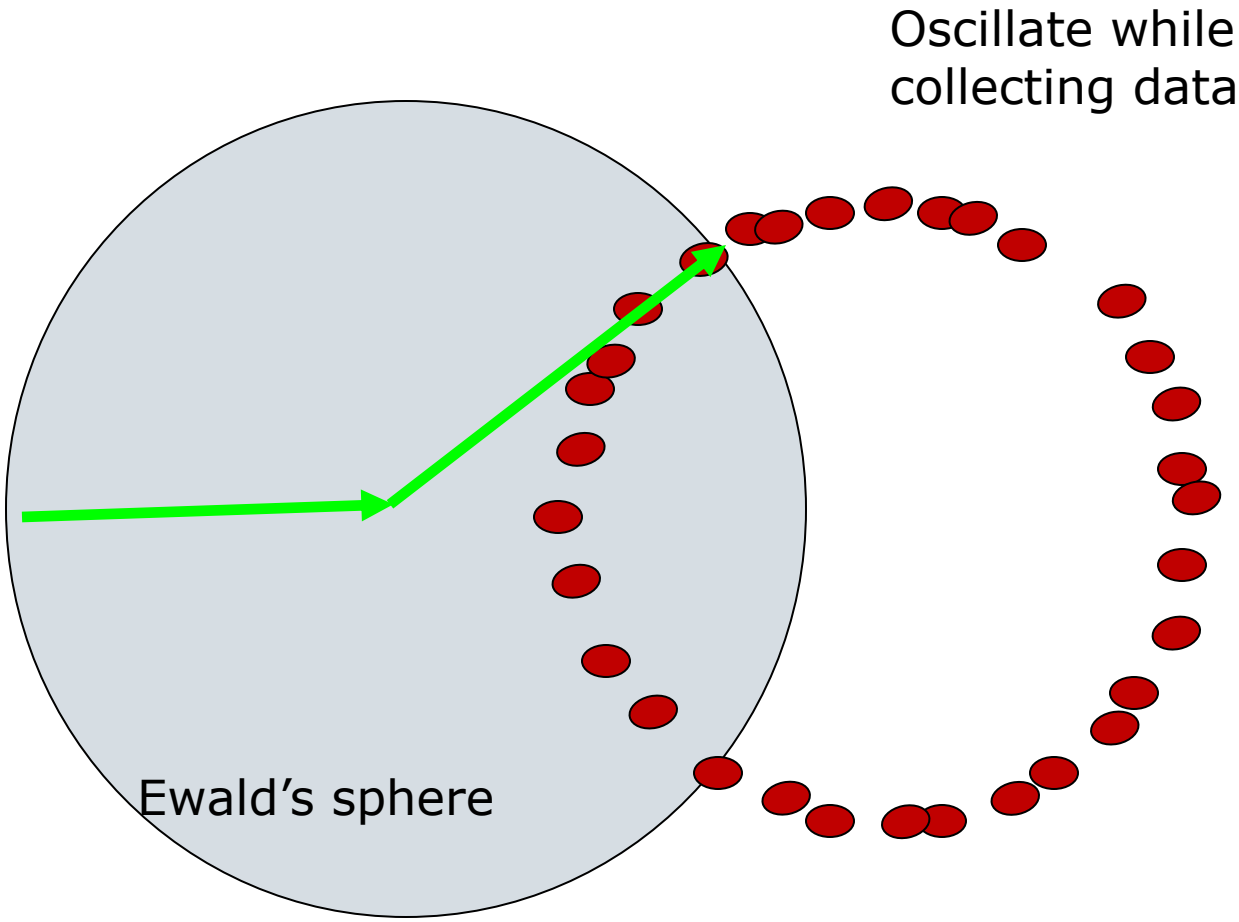


- Just 1 angle (detector)
- Bragg's law sufficient
- If large area detector → 0 angles
  - Very useful for fast/time dependent measurements

Powder Diffractometer with an Area Detector

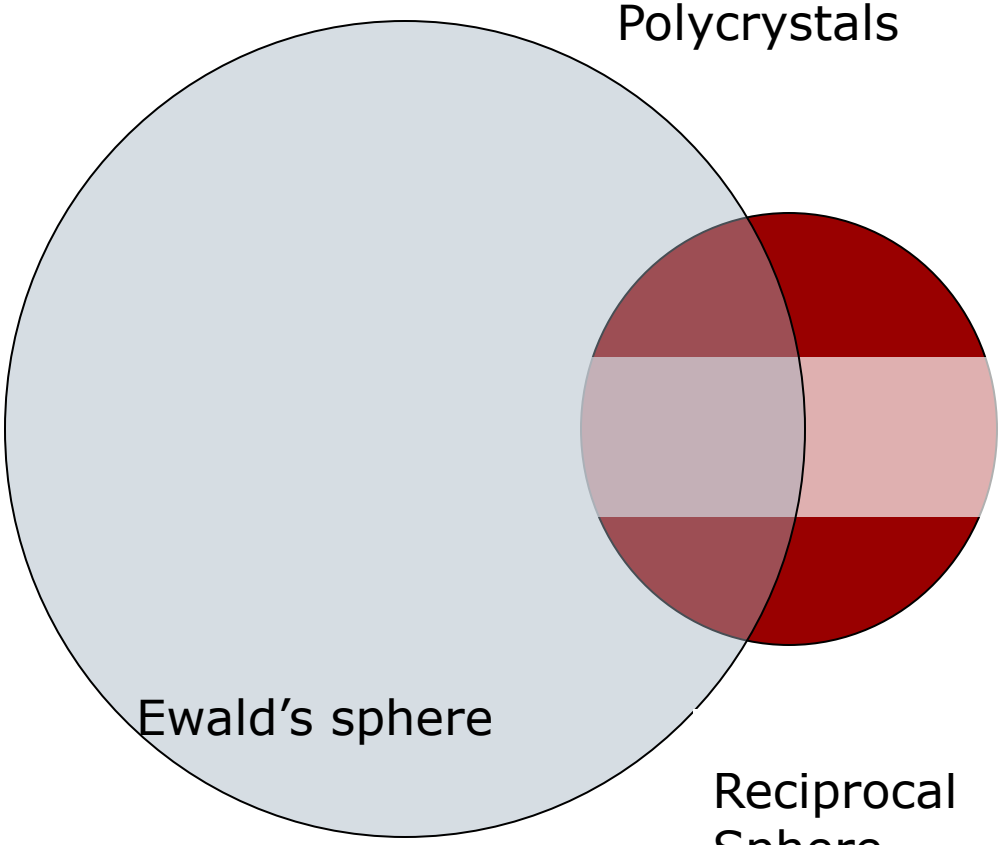


Powder Average and Rocking



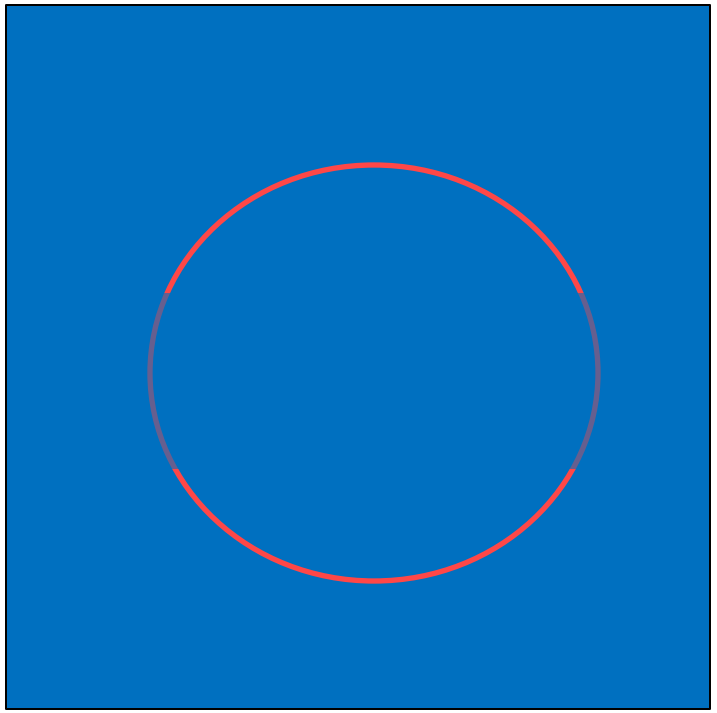
Texture

Oriented
Polycrystals



Reciprocal
Sphere

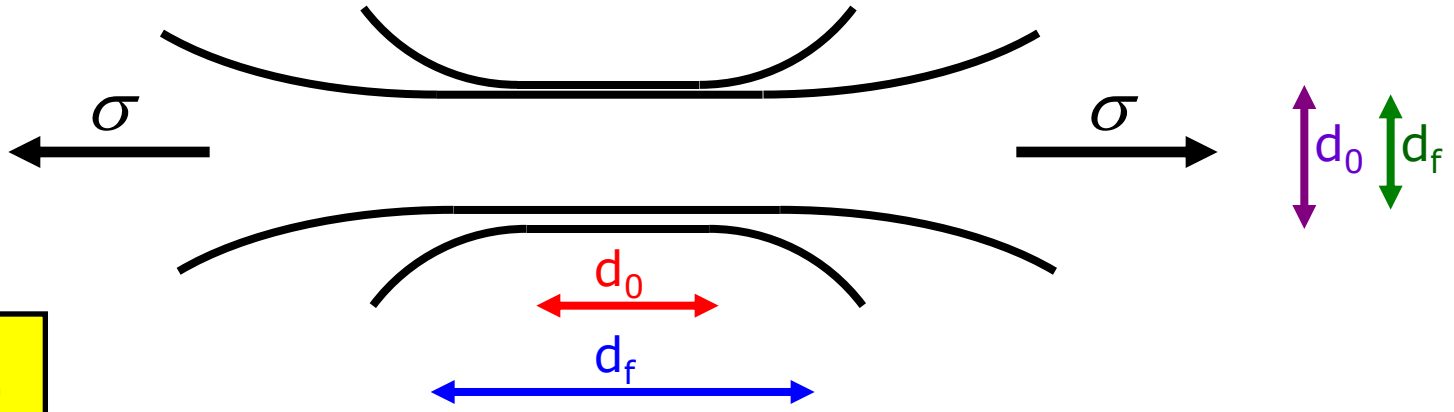
Diffraction pattern



Partial diffraction ring

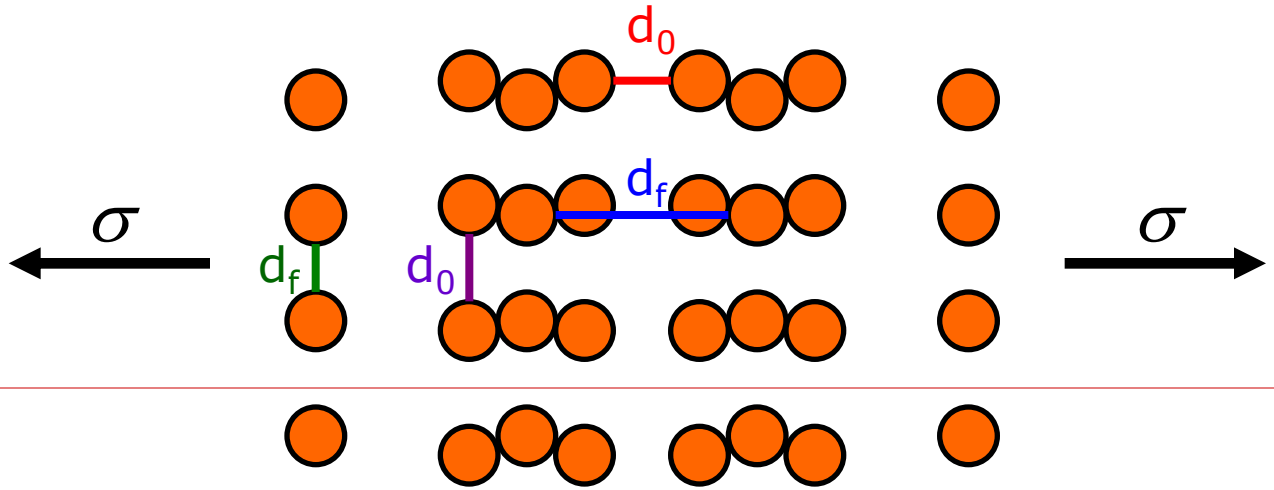
Strain

Global Scale



$$\varepsilon = \frac{d_f - d_0}{d_0}$$

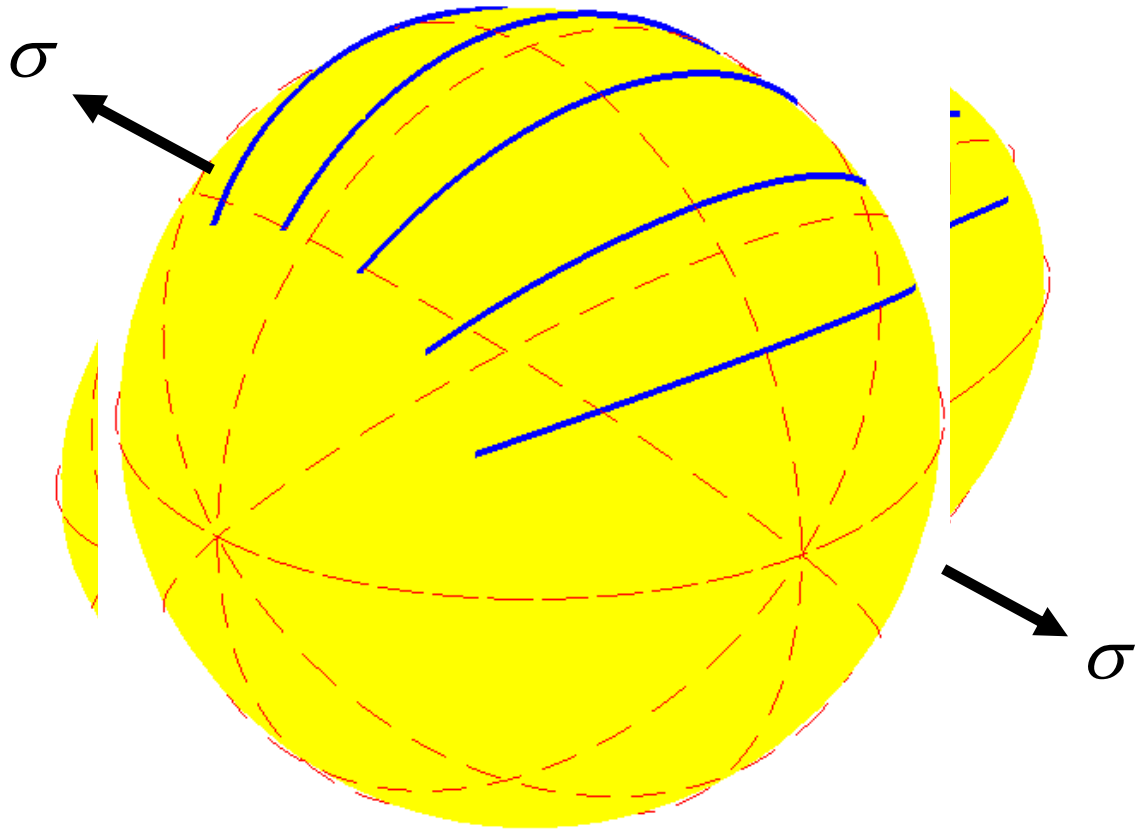
Local Scale



Strain in Polycrystals

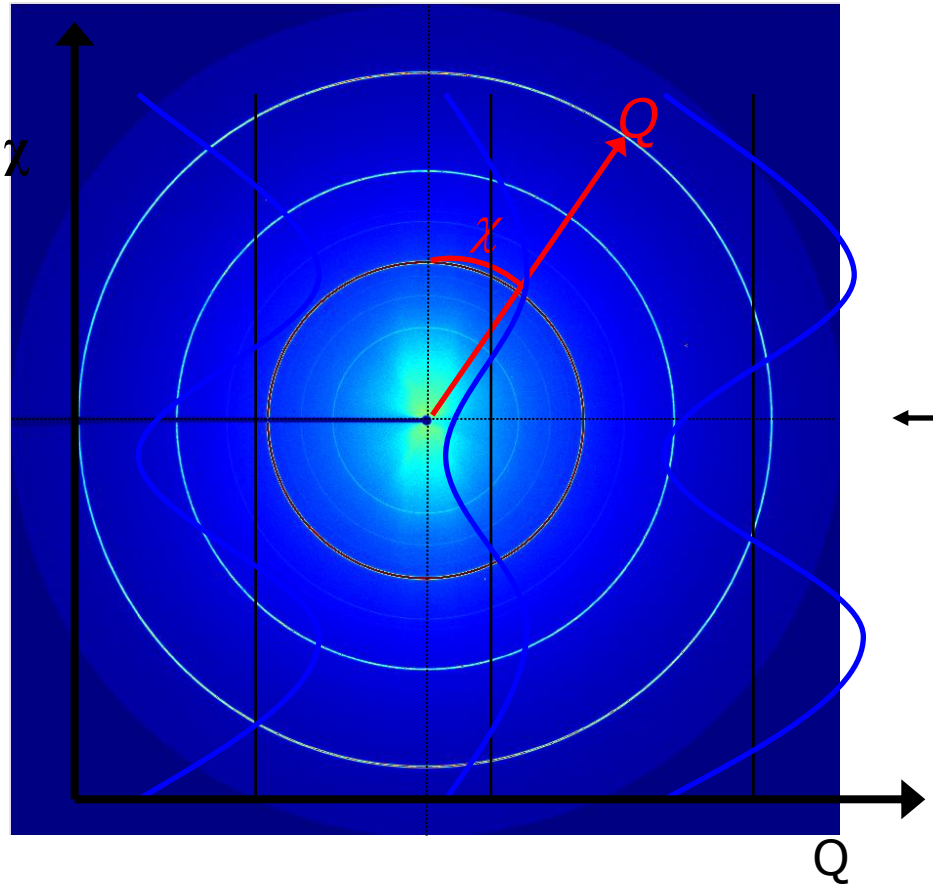
$$\bar{u}_i = \epsilon_{ij} k_{0_j}$$

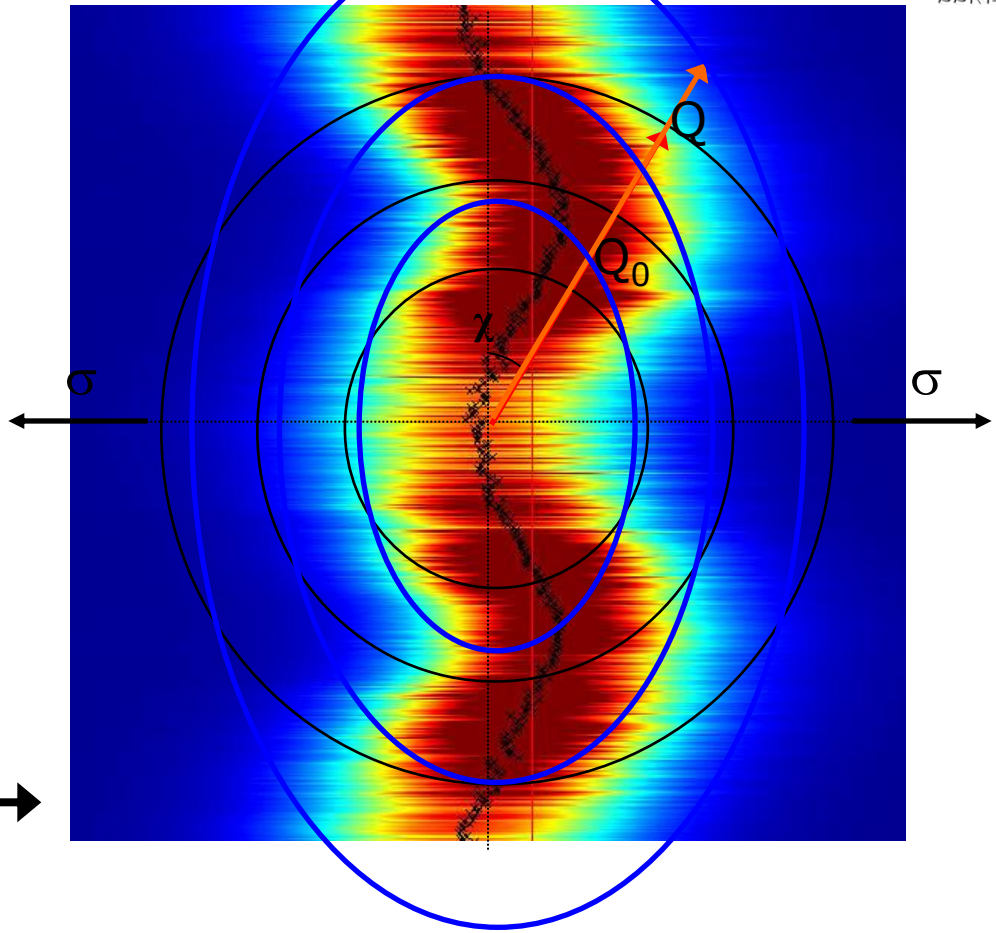
Reciprocal Sphere



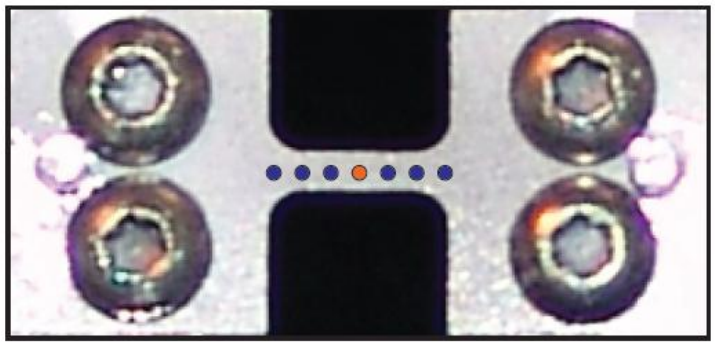
Strain Ellipsoid

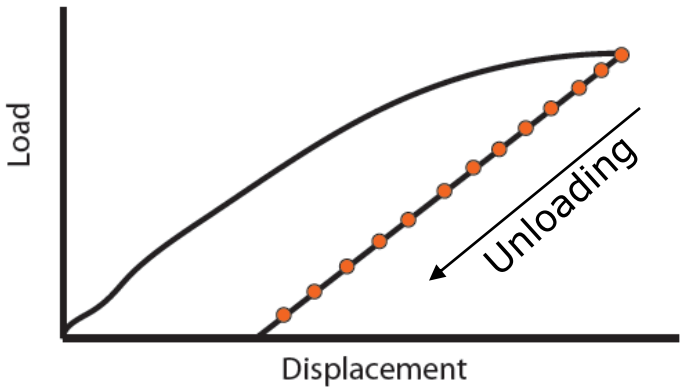
Coordinate Transformation



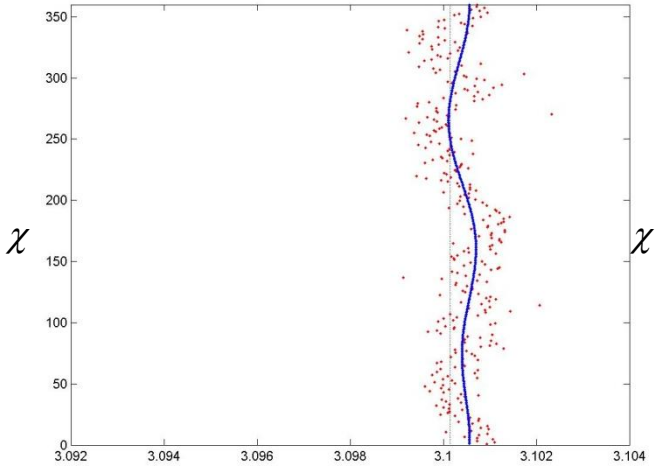


Strain Relaxation

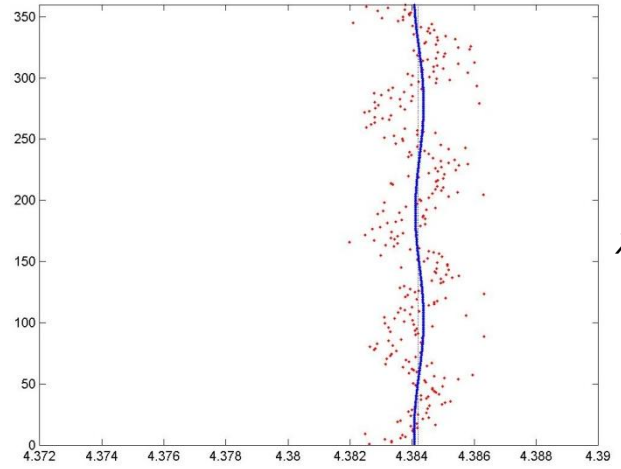




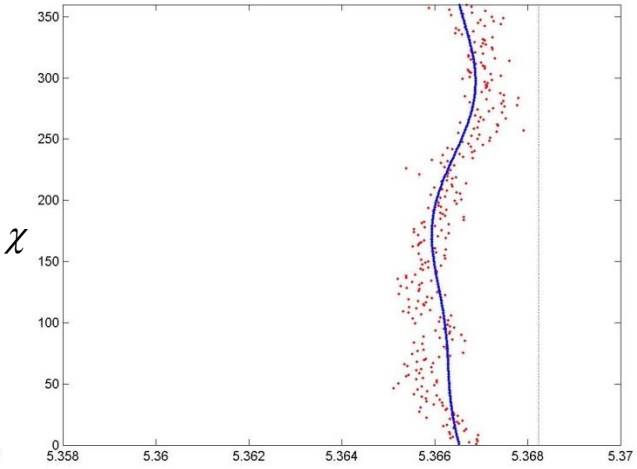
110



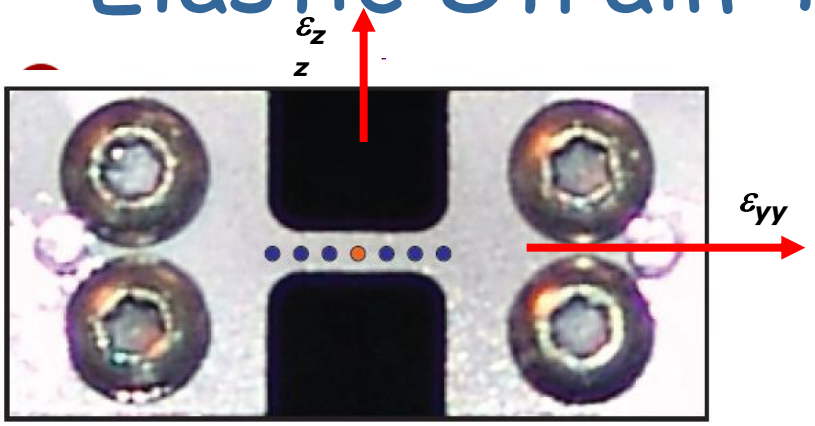
200

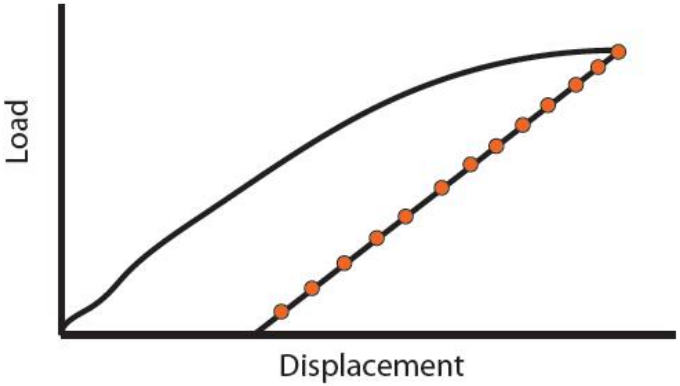


211



Elastic Strain Tensor: bcc Fe

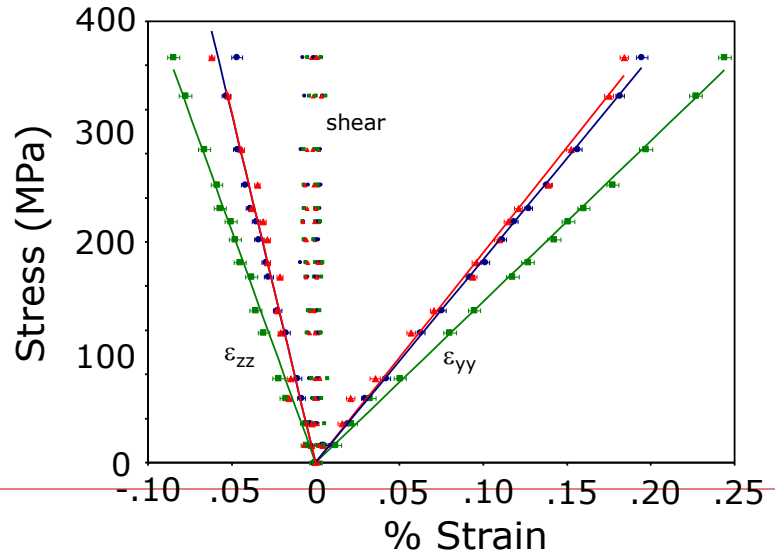


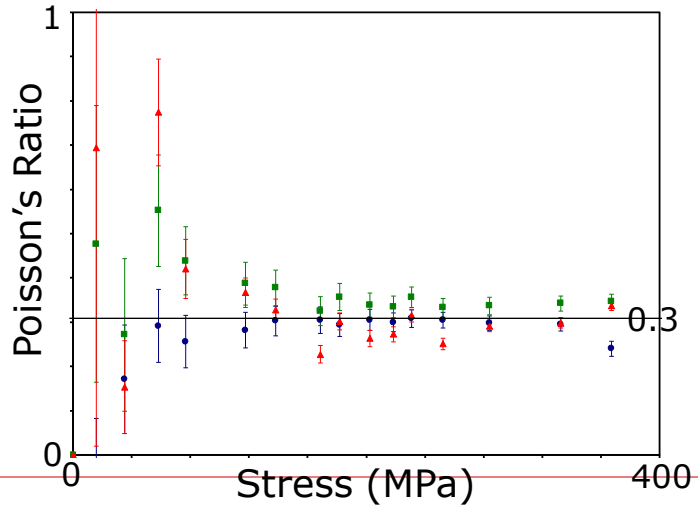


110 E_m = 211 GPa

200 E_m = 167 GPa

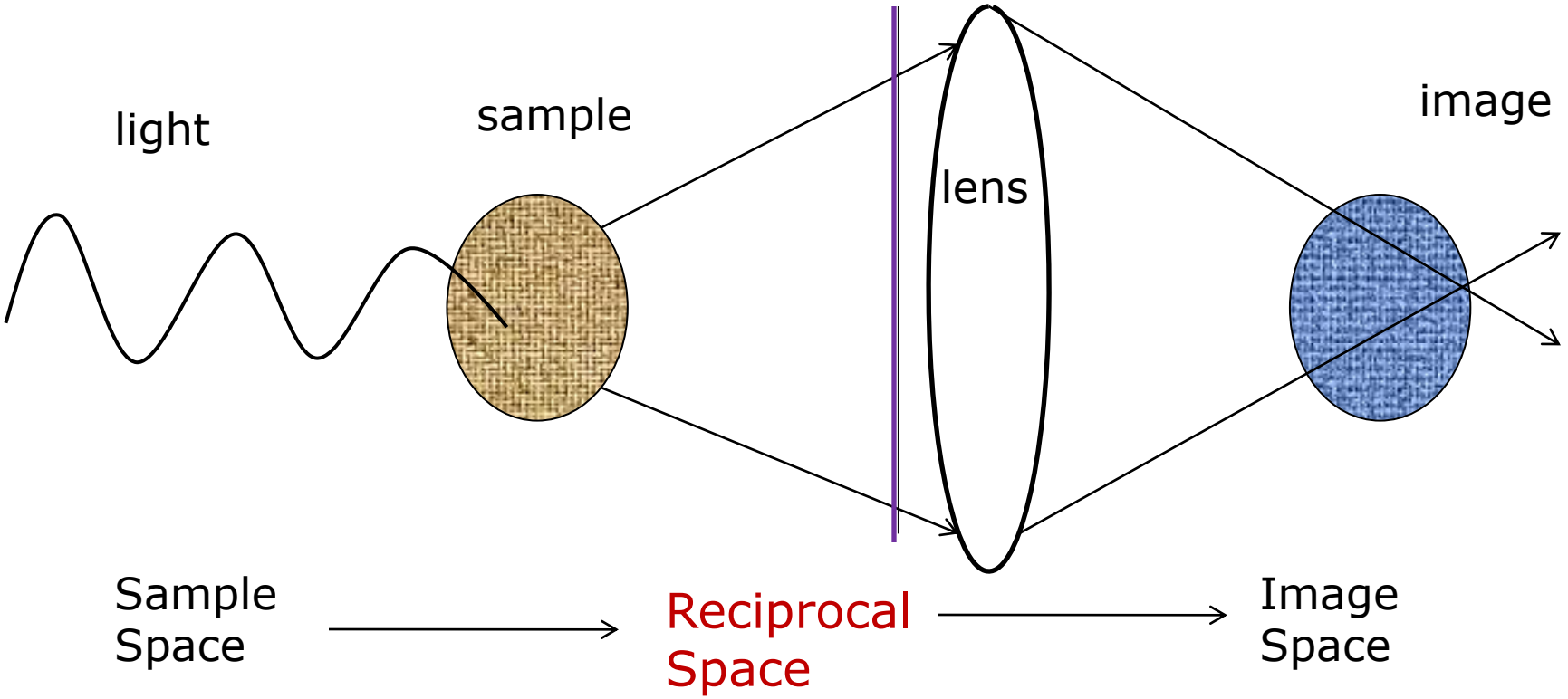
211 E_m = 218 GPa





Scattering Physics

X-ray lens with resolution better than ~10nm don't exist



X-ray Scattering/diffraction is about probing the structure without a lens

Thanks

- Reciprocal Space is the map of diffraction pattern

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