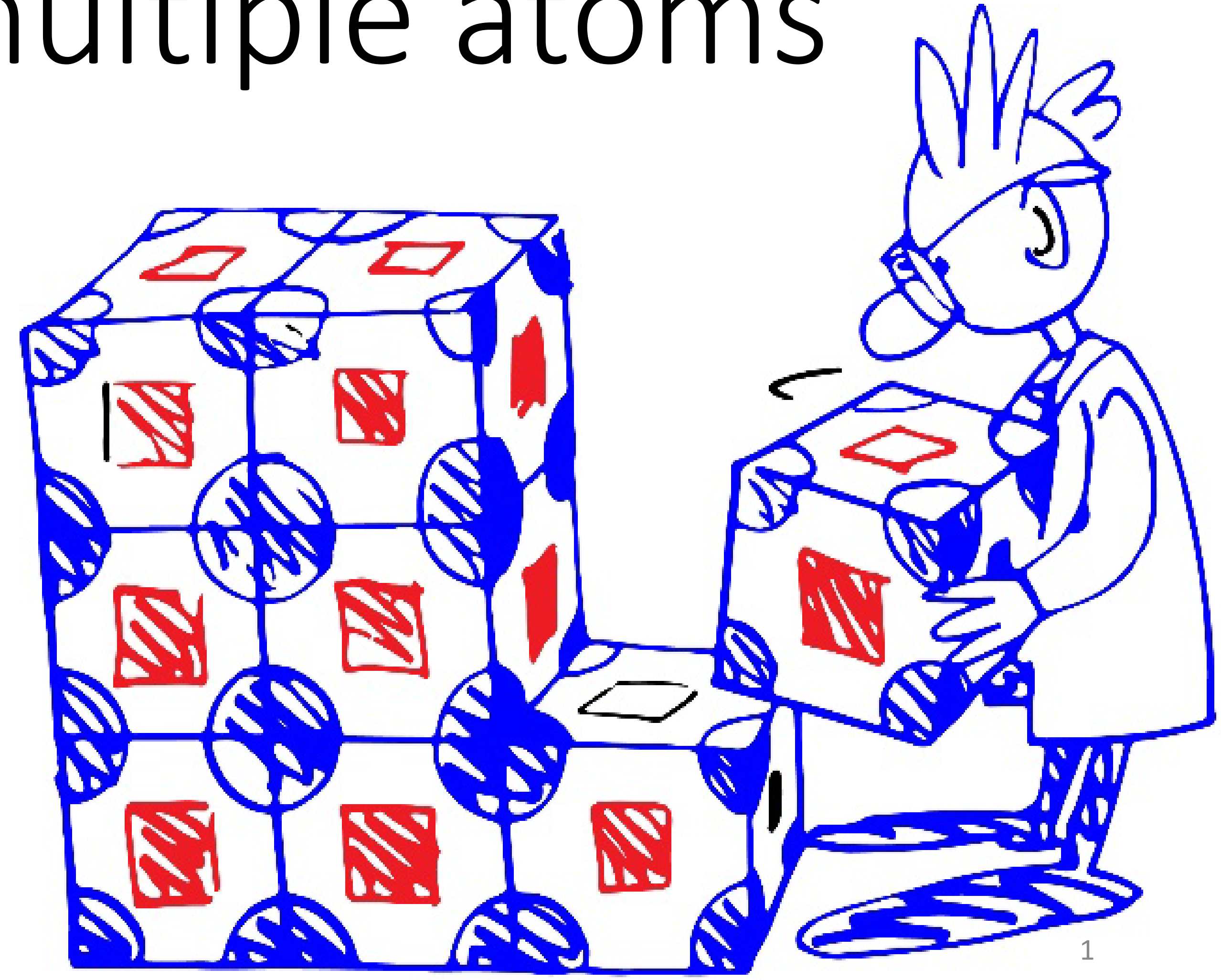
Scattering from multiple atoms

Diffraction from a crystal



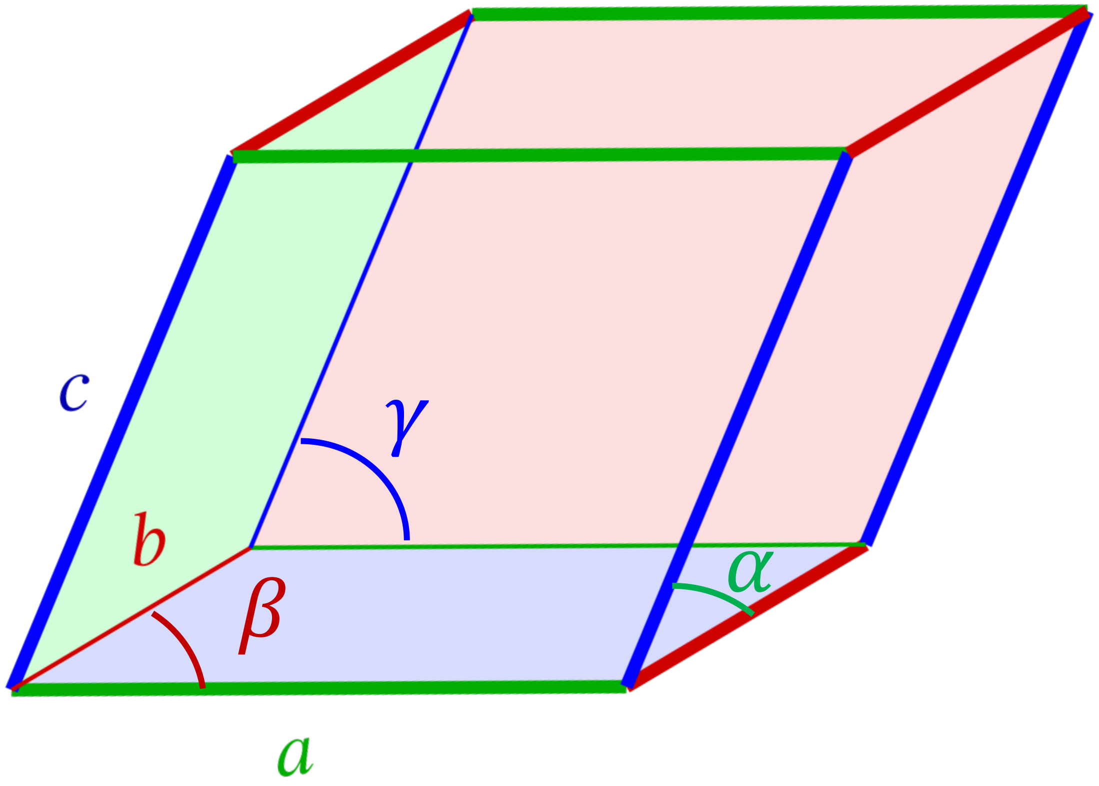
We start with a generic paralepidid

The shape of our ‘box’ is determined by 6 parameters known as the **lattice parameters**.

These determine the **unit cell** and also help us think about diffraction.

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma$



Miller indices

Procedure for drawing a crystallographic planes

1. The indices in (*hkl*) define the plane.
2. Find the intercepts of a plane with the cell parameters *a, b, c.*
3. Take the reciprocal of the fractions to get the Miller indices.

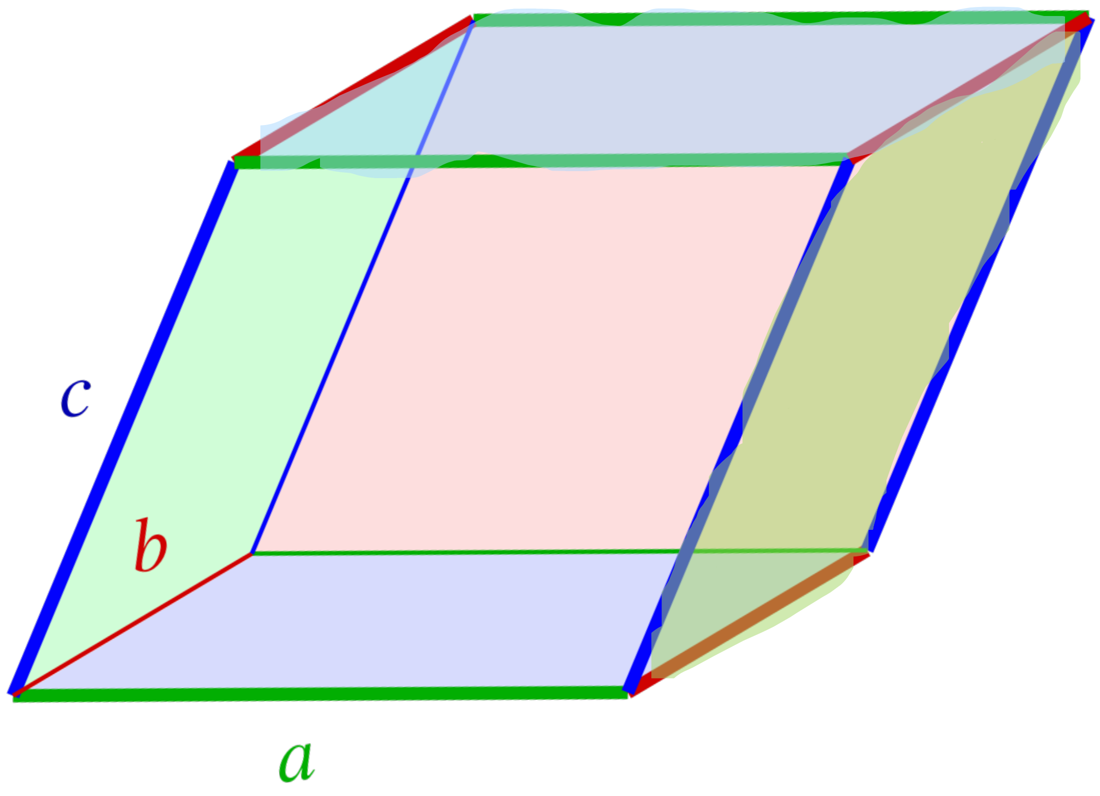
$$\frac{1}{h}a \qquad \frac{1}{k}b \qquad \frac{1}{l}c$$

Other notes:

- They are not the same thing as zone axis, which is given by **[*uvw*]** , note the square brackets.
- We indicate Miller indices by three whole numbers and the symbols **(*hkl*)**

Labeling the faces of our unit cell

Find the (100), (010) and (001) faces.



$$\frac{1}{h}a \qquad \frac{1}{k}b \qquad \frac{1}{l}c$$

$$\frac{1}{1}a \qquad \frac{1}{0}b \qquad \frac{1}{0}c$$

$$1\,a \qquad \infty b \qquad \infty c$$

$$\frac{1}{0}a \qquad \frac{1}{0}b \qquad \frac{1}{1}c$$

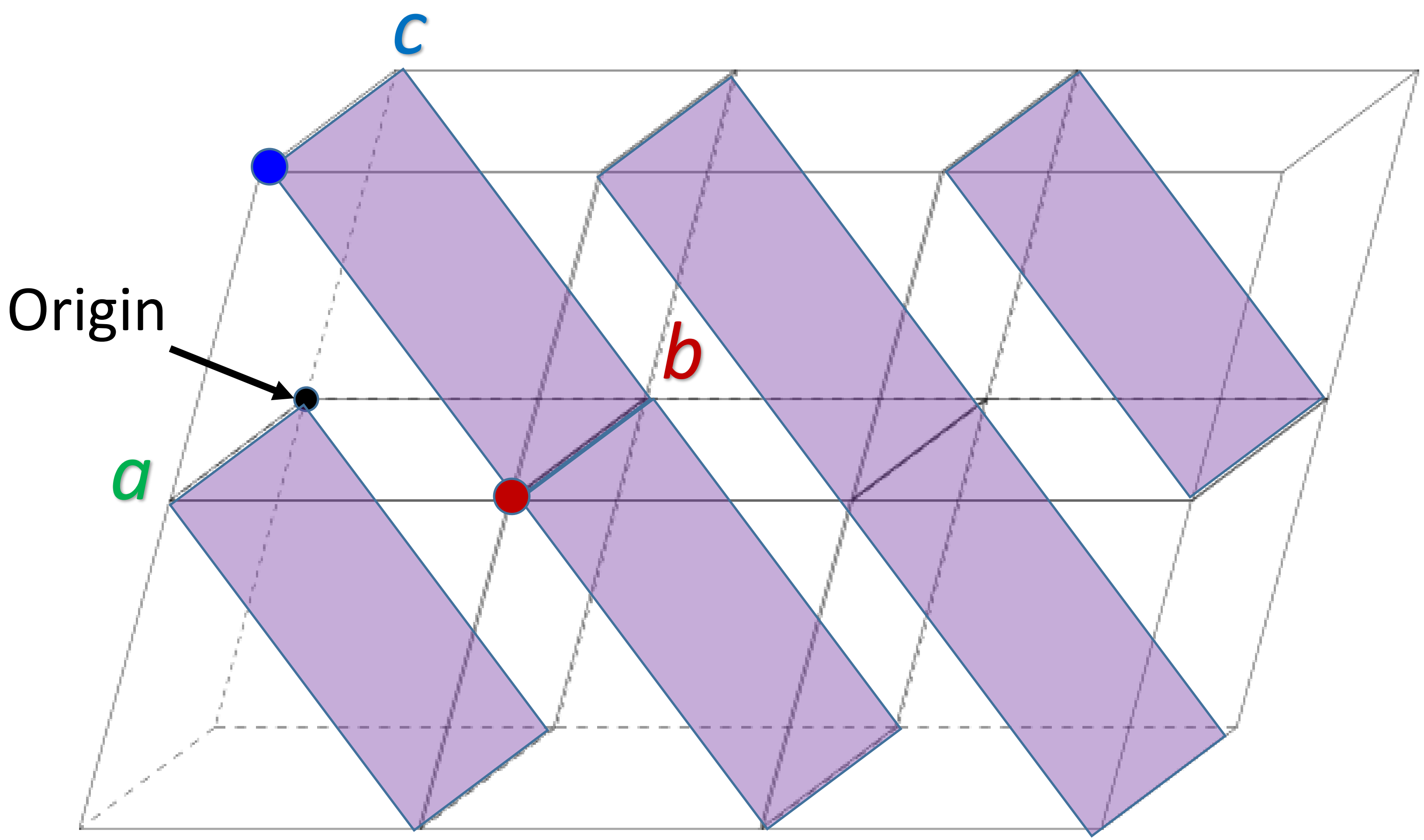
$$\infty\,a \qquad \infty b \qquad 1\,c$$

Crystallographic planes beyond the unit cell

Find the
(011) planes

$$\frac{1}{h}a \quad \frac{1}{k}b \quad \frac{1}{l}c$$

$$\frac{1}{0}a \quad \frac{1}{1}b \quad \frac{1}{1}c$$

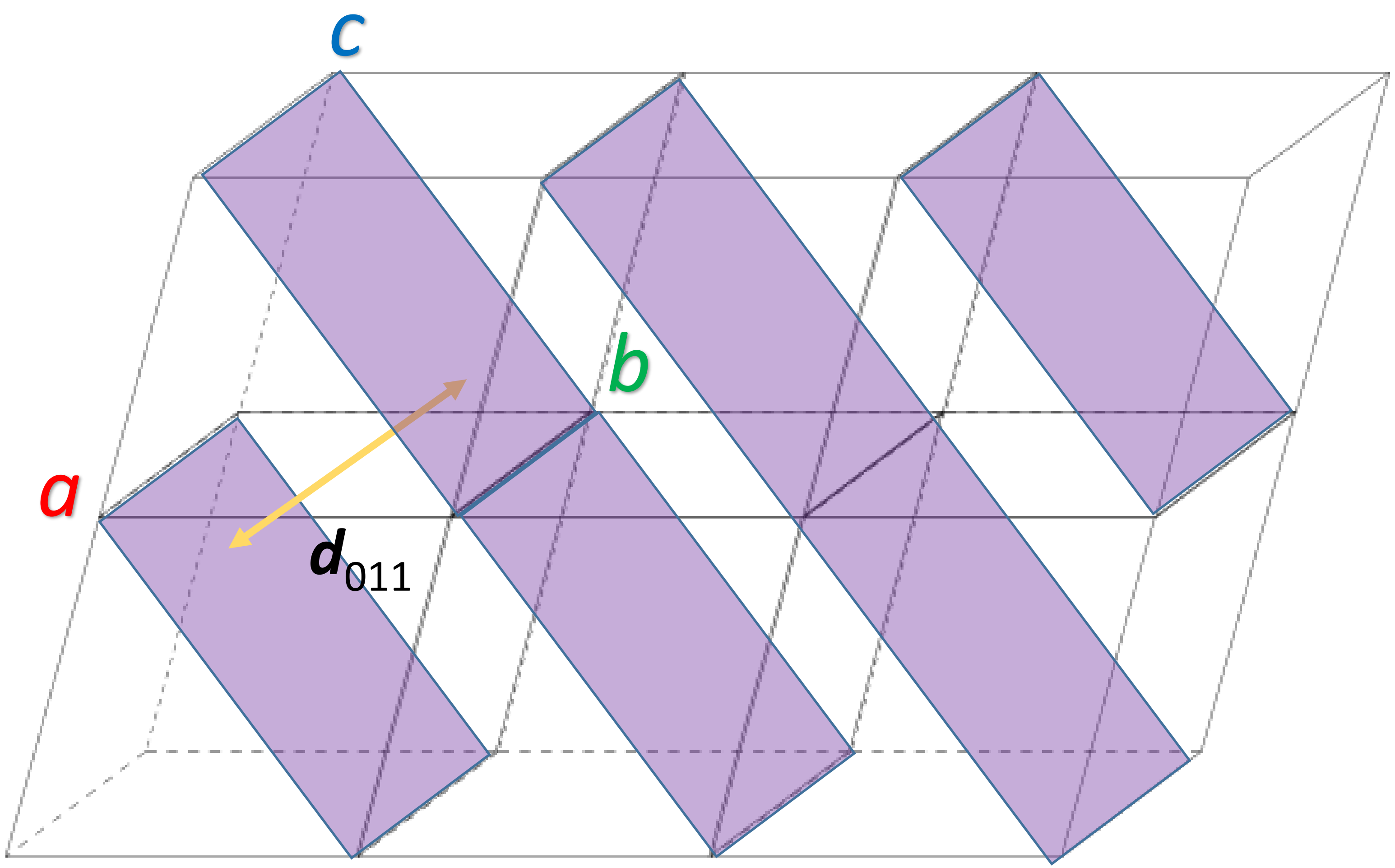


Crystallographic planes beyond the unit cell

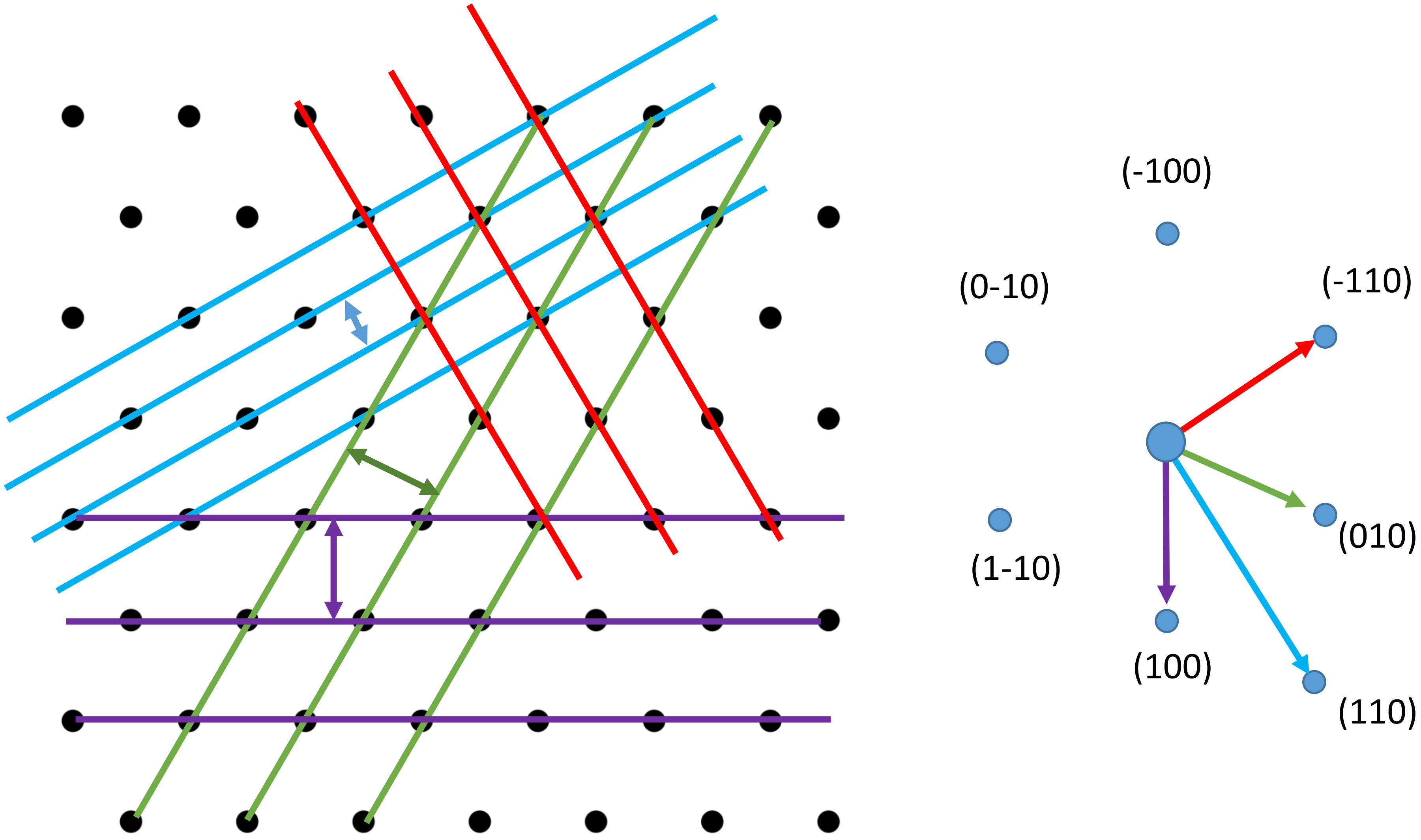
From the (011) planes, let's find the vector $\boldsymbol{G}^*_{011}$

First find the spacing between the planes, which we call the d-spacing.

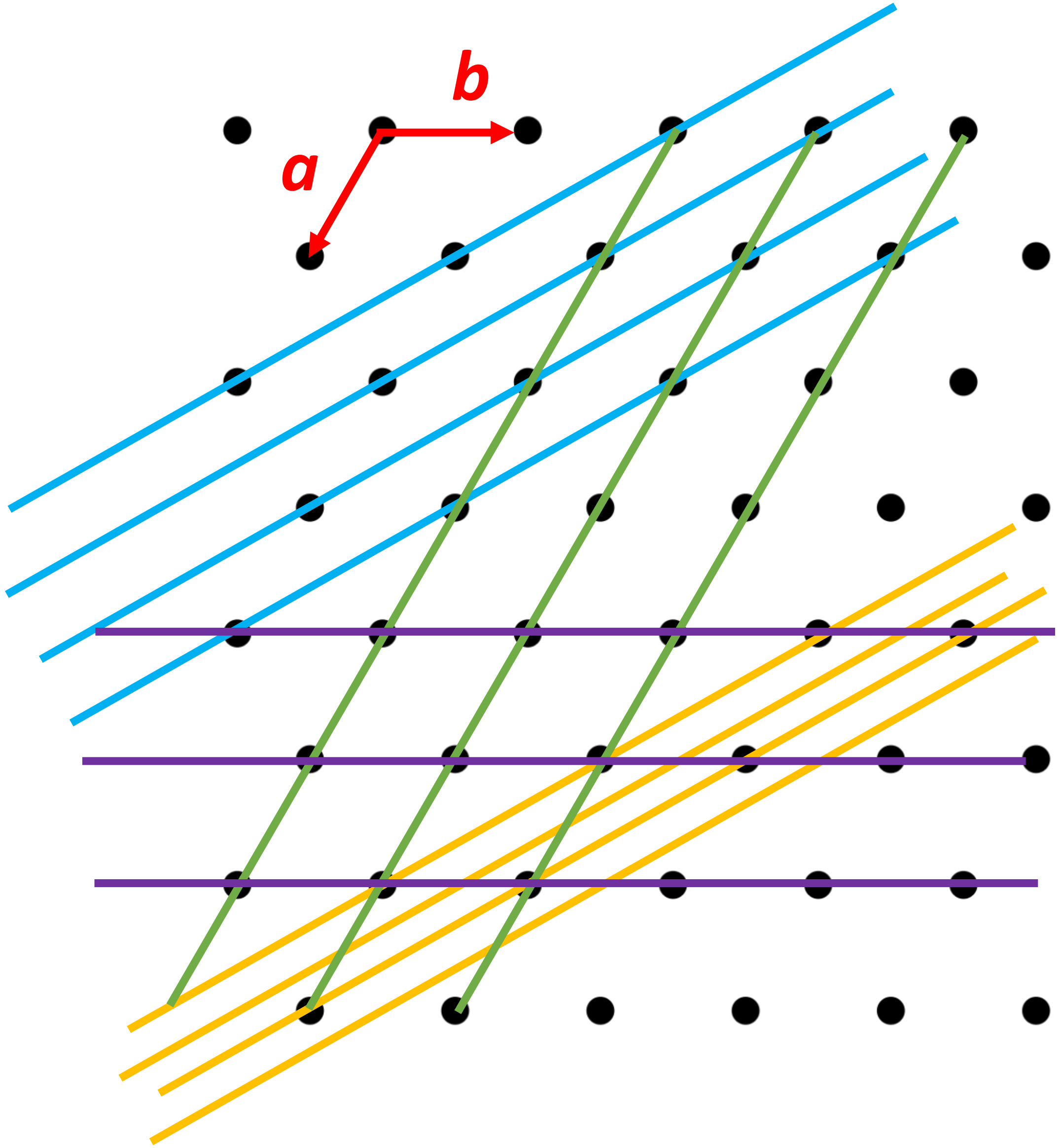
$$\boldsymbol{G}^*_{hkl} = \frac{2\pi}{\boldsymbol{d}_{hkl}}$$



Building the reciprocal lattice

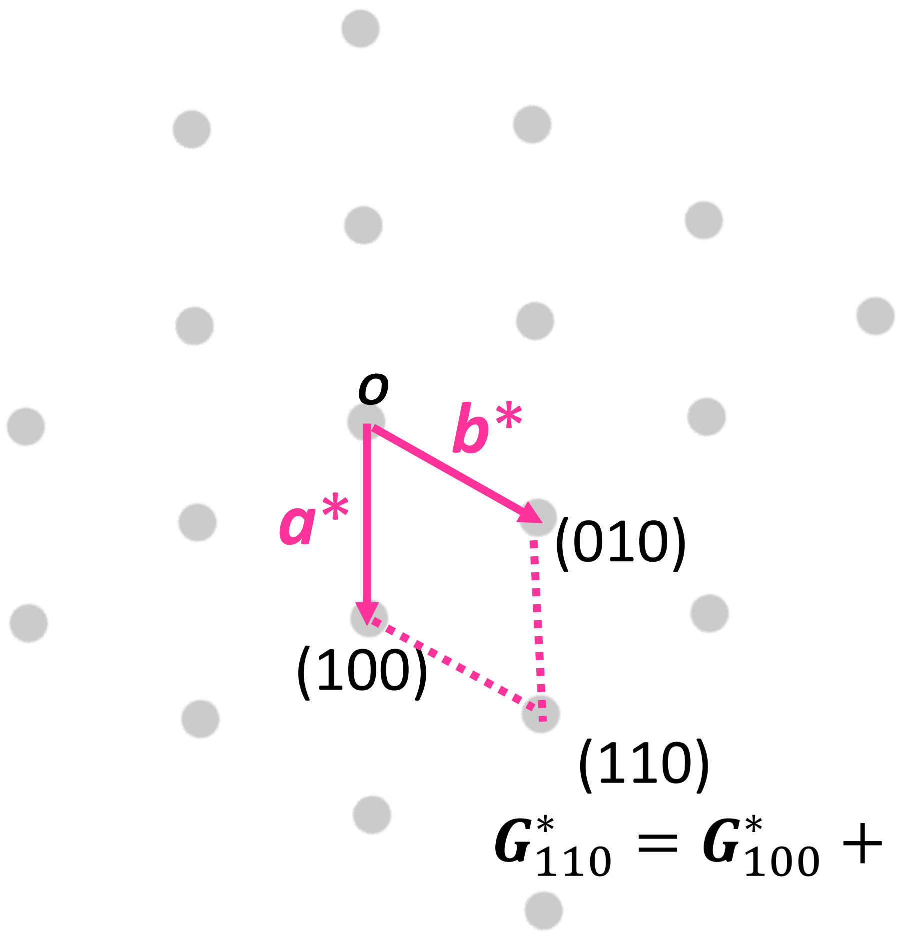


Real space lattice



Reciprocal space lattice

$$\boldsymbol{G}^*_{hkl} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$

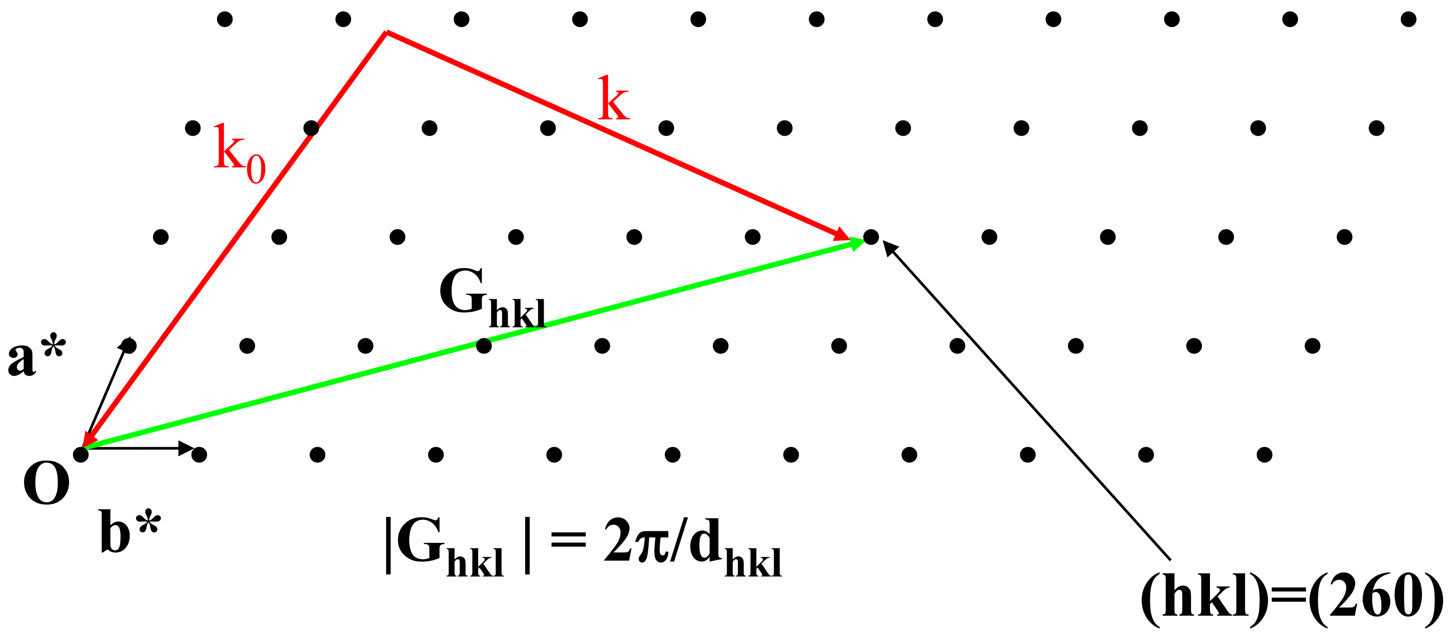


$$\boldsymbol{G}^*_{110} = \boldsymbol{G}^*_{100} + \boldsymbol{G}^*_{010}$$

Diffraction and Bragg's law

G_{hkl} is called a reciprocal lattice vector (node denoted hkl)

h, k and l are called Miller indices



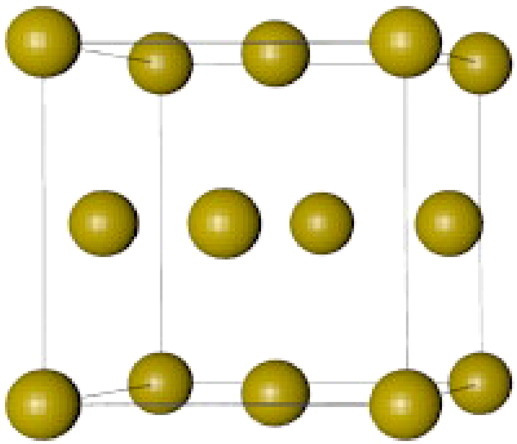
$$\vec{G}_{hkl} = \vec{Q}$$

$$\frac{2\pi n}{d_{hkl}} = \frac{4\pi \sin\theta}{\lambda}$$

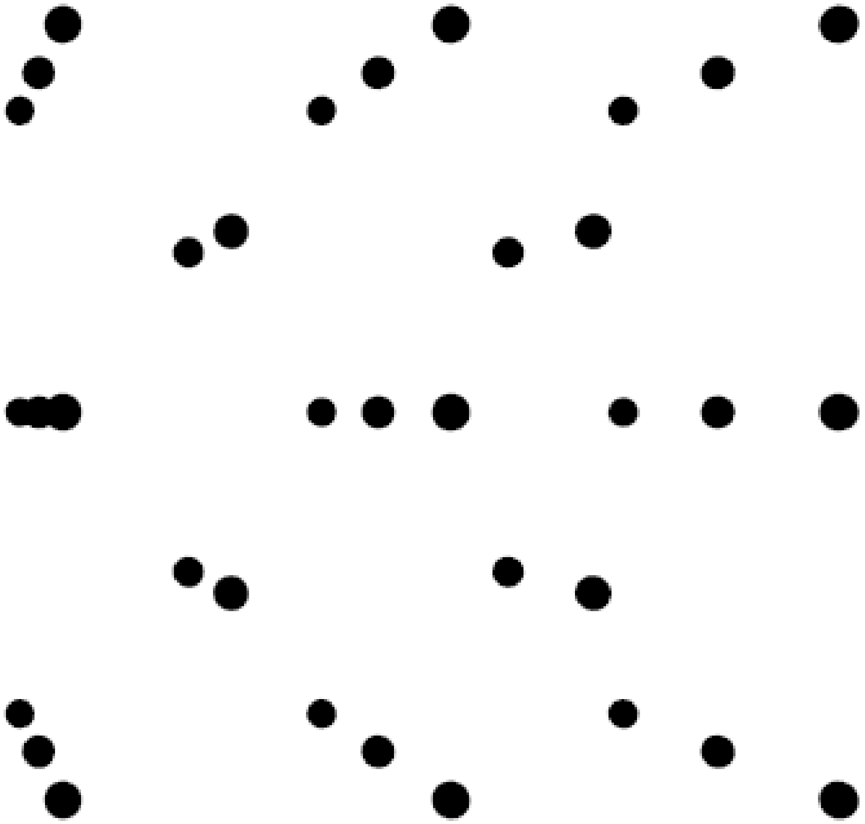
$$n\lambda = 2d_{hkl} \sin\theta$$

Relationship between real and reciprocal space

Real Space

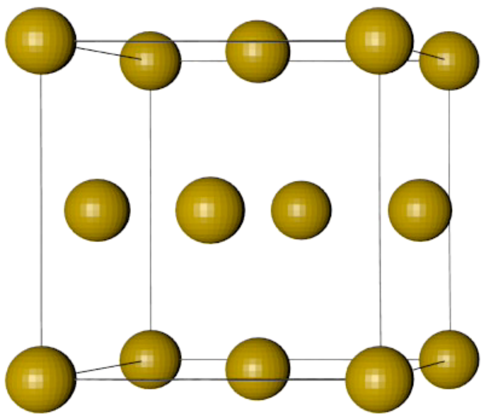


Reciprocal Space

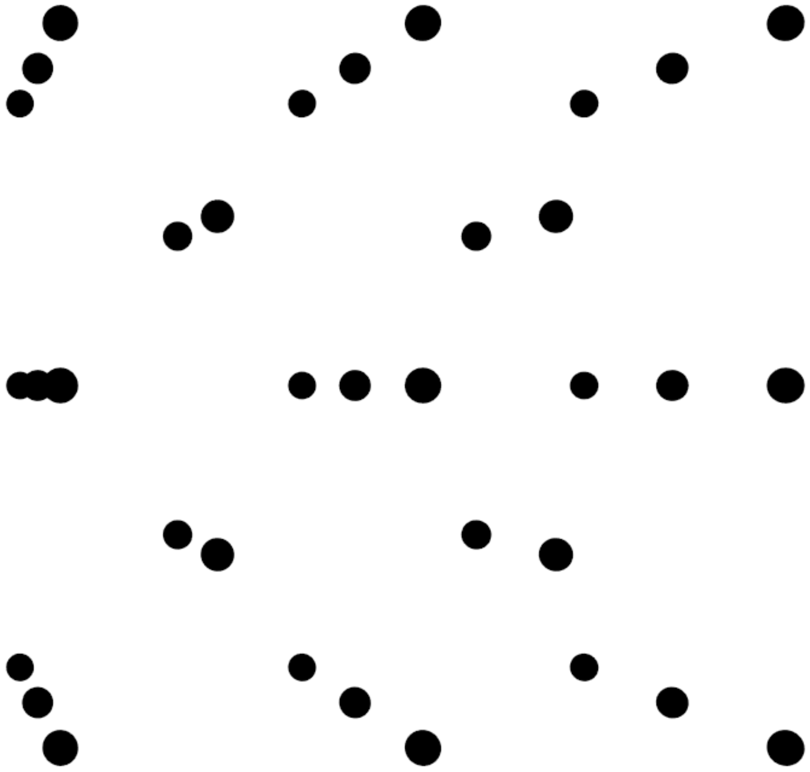


Beam of neutrons or x-rays scattered from planes

Real Space

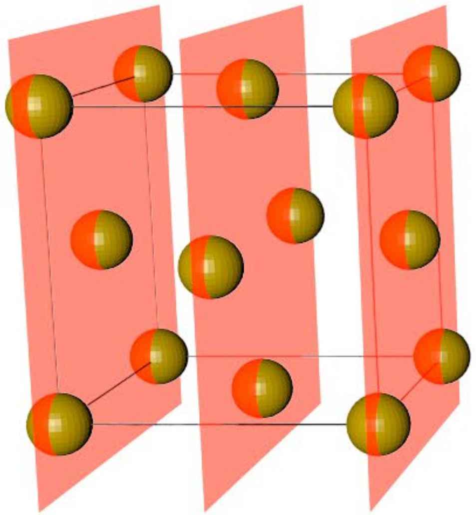


Reciprocal Space

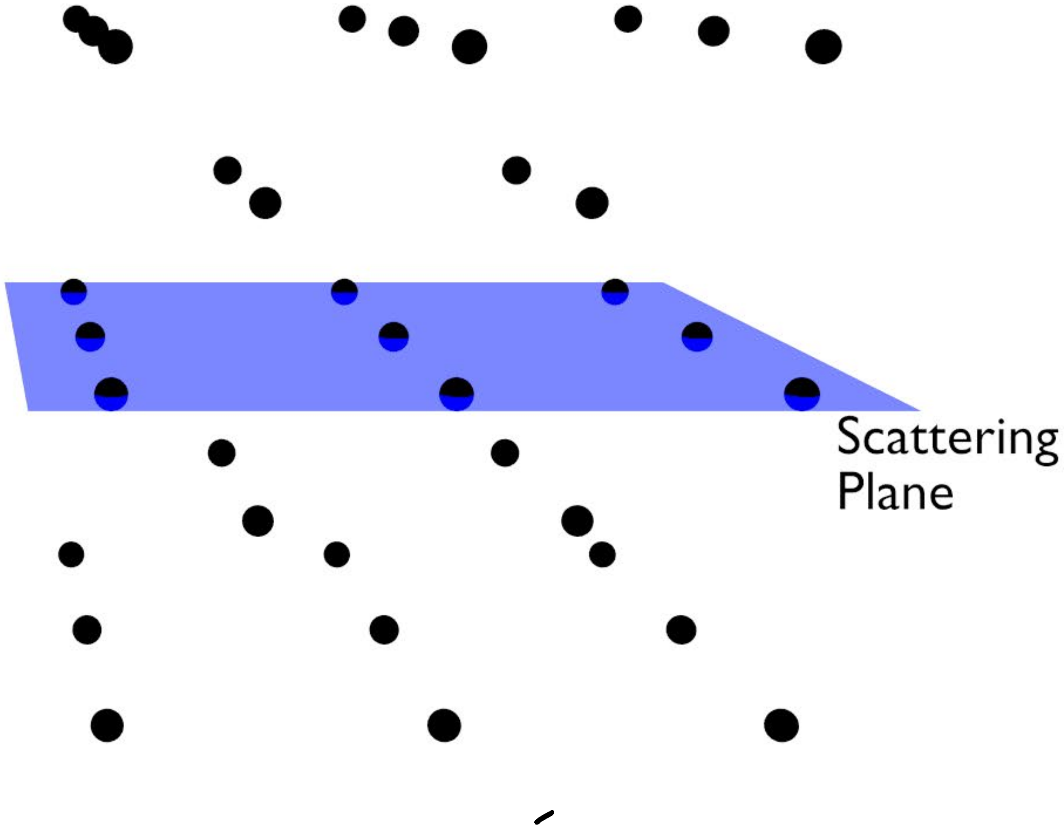


Bragg reflections from crystallographic planes

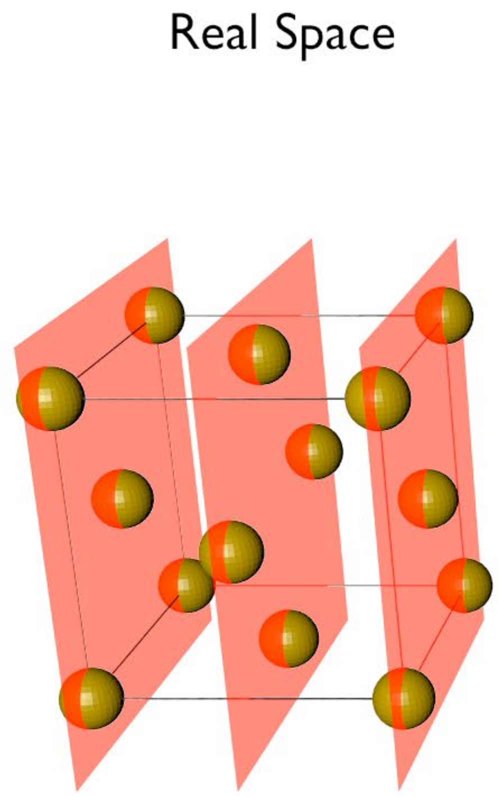
Real Space

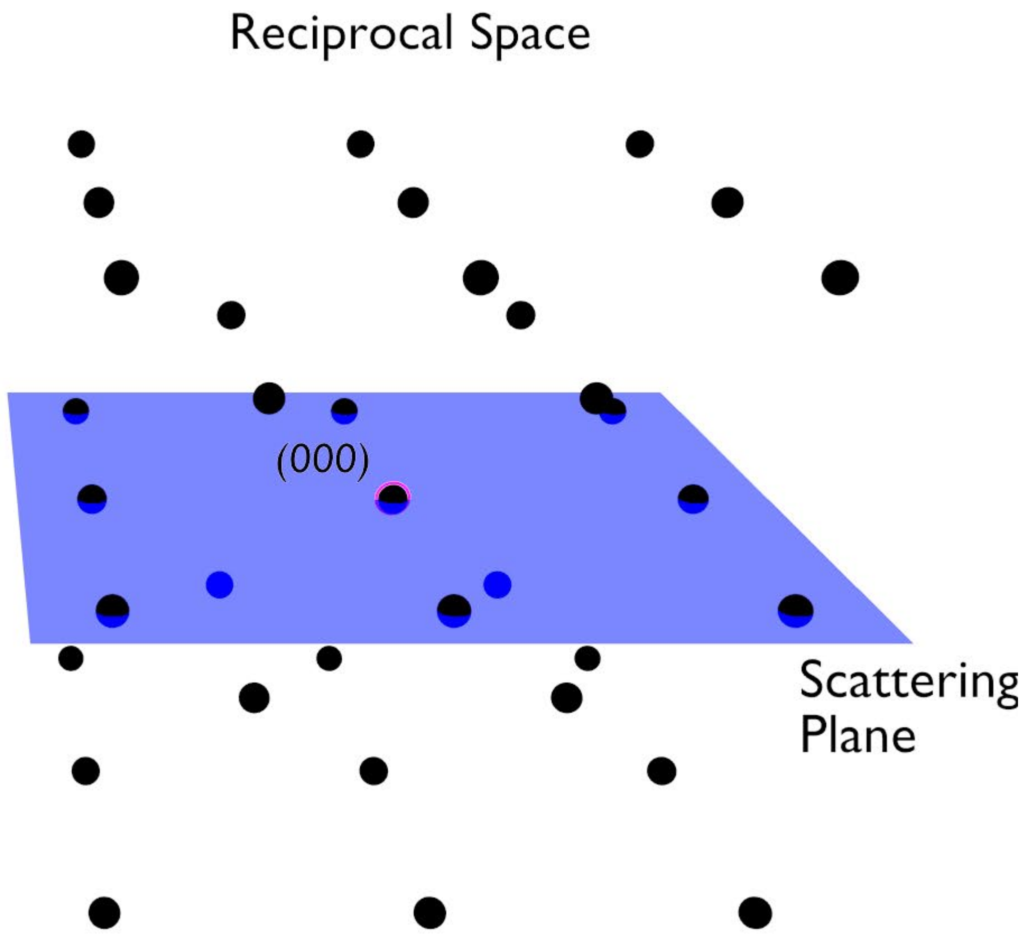


Reciprocal Space



Centering operations lead to systematic absences

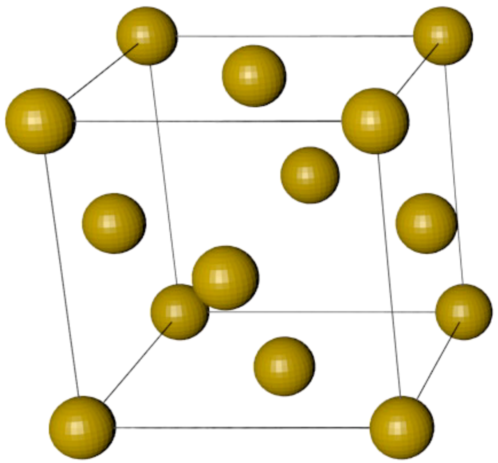




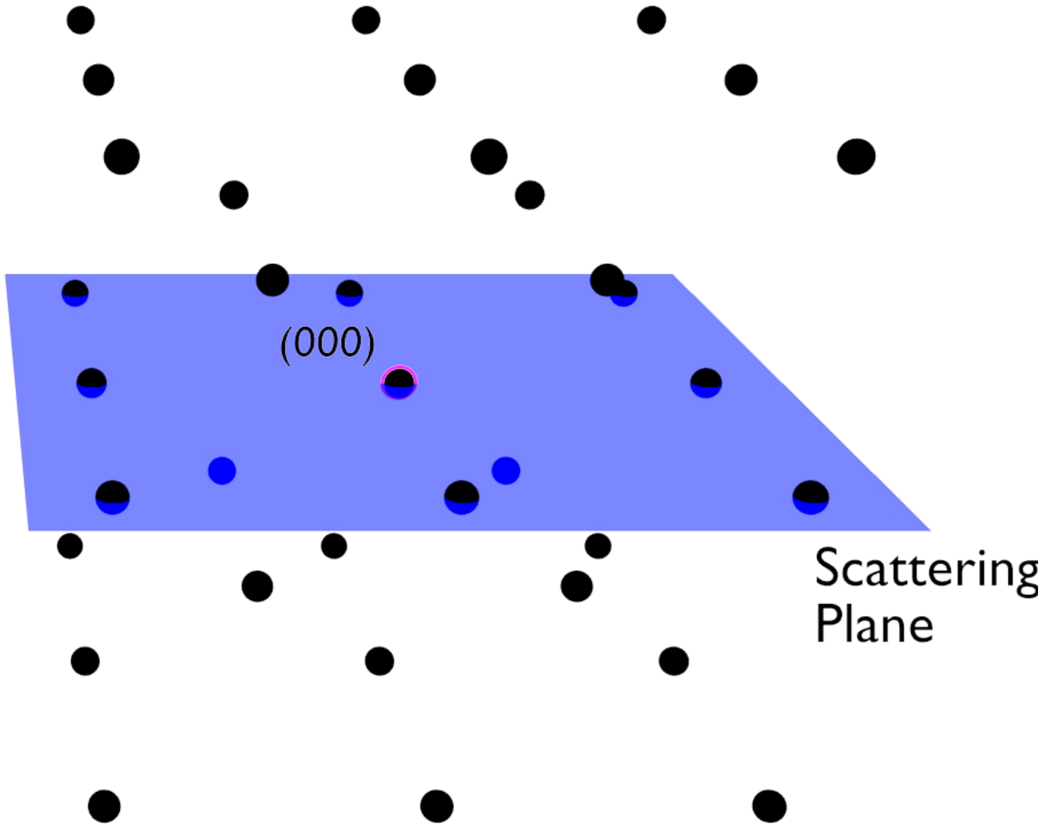
{001} family of planes are systematically absent

Other allowed reflections in fcc lattice

Real Space



Reciprocal Space



Ewald sphere for different wavelengths

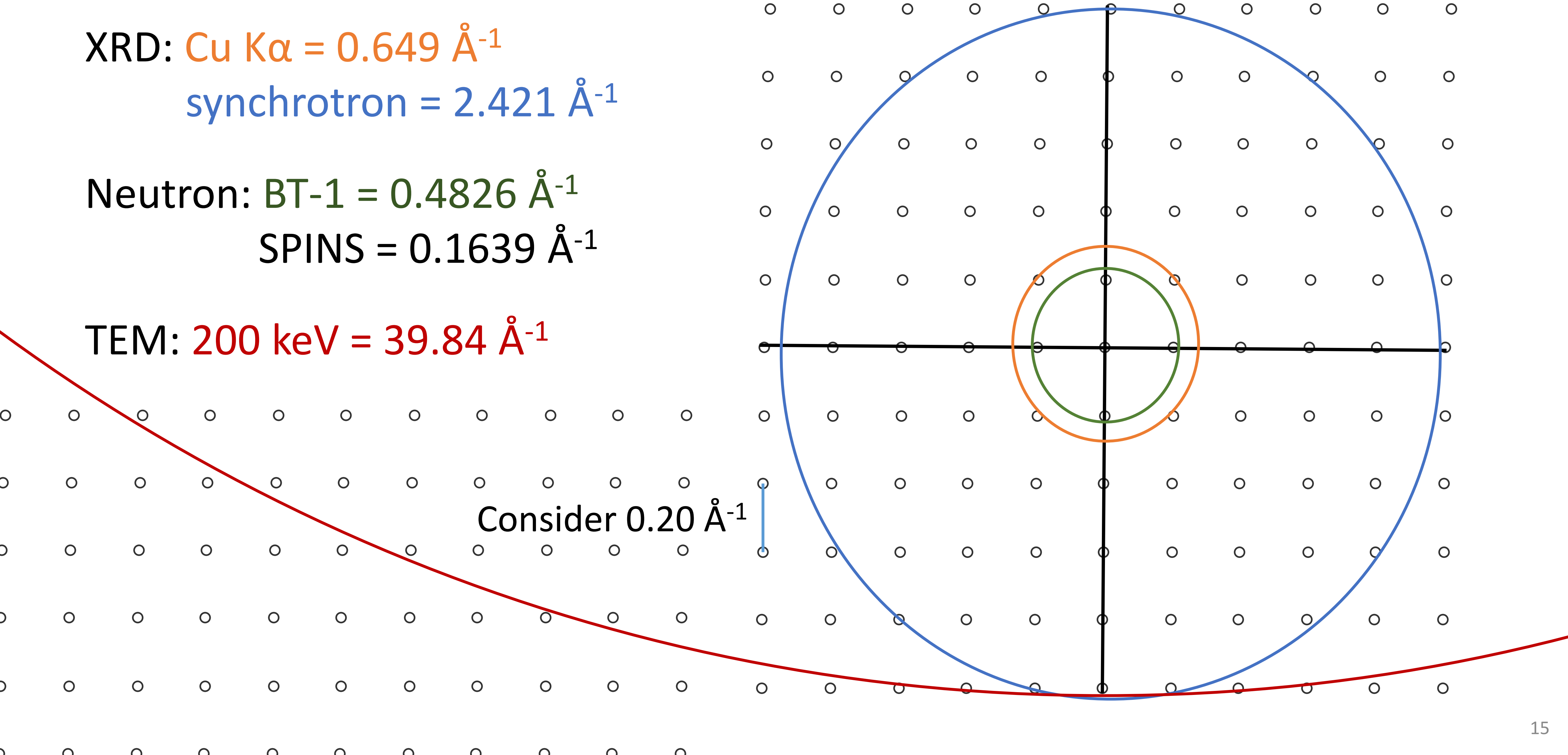
XRD: Cu Kα = 0.649 $Å^{-1}$

synchrotron = 2.421 $Å^{-1}$

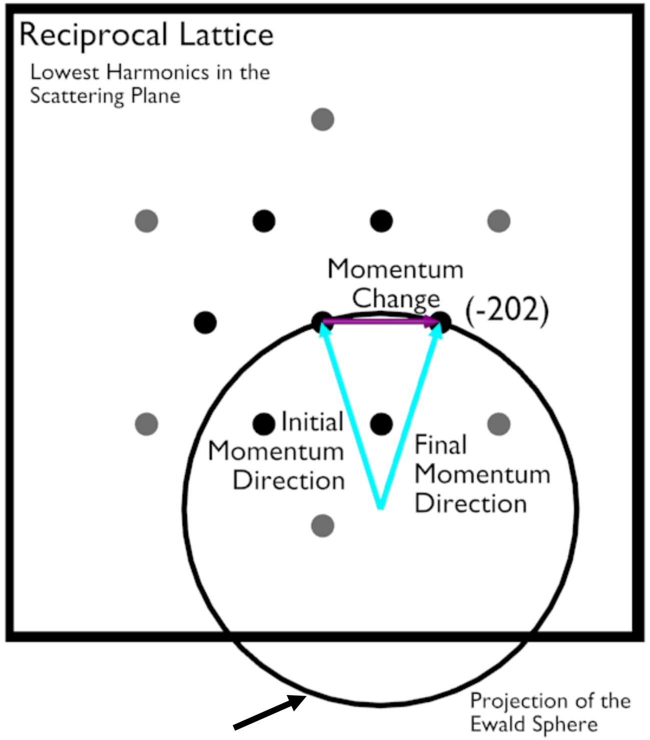
Neutron: BT-1 = 0.4826 $Å^{-1}$

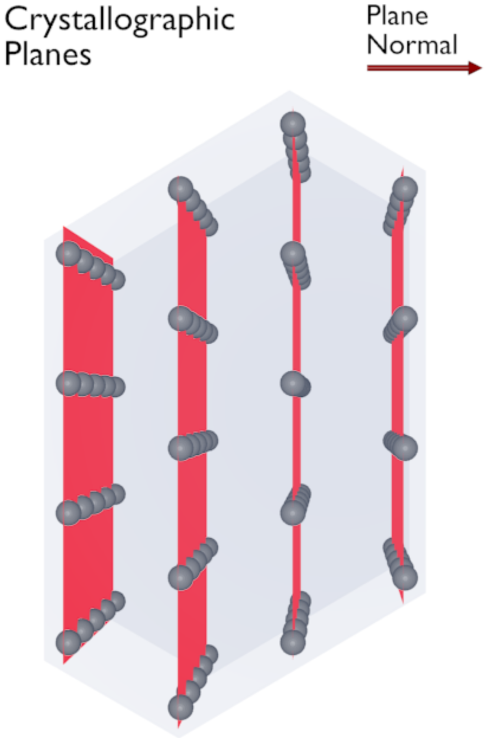
SPINS = 0.1639 $Å^{-1}$

TEM: 200 keV = 39.84 $Å^{-1}$



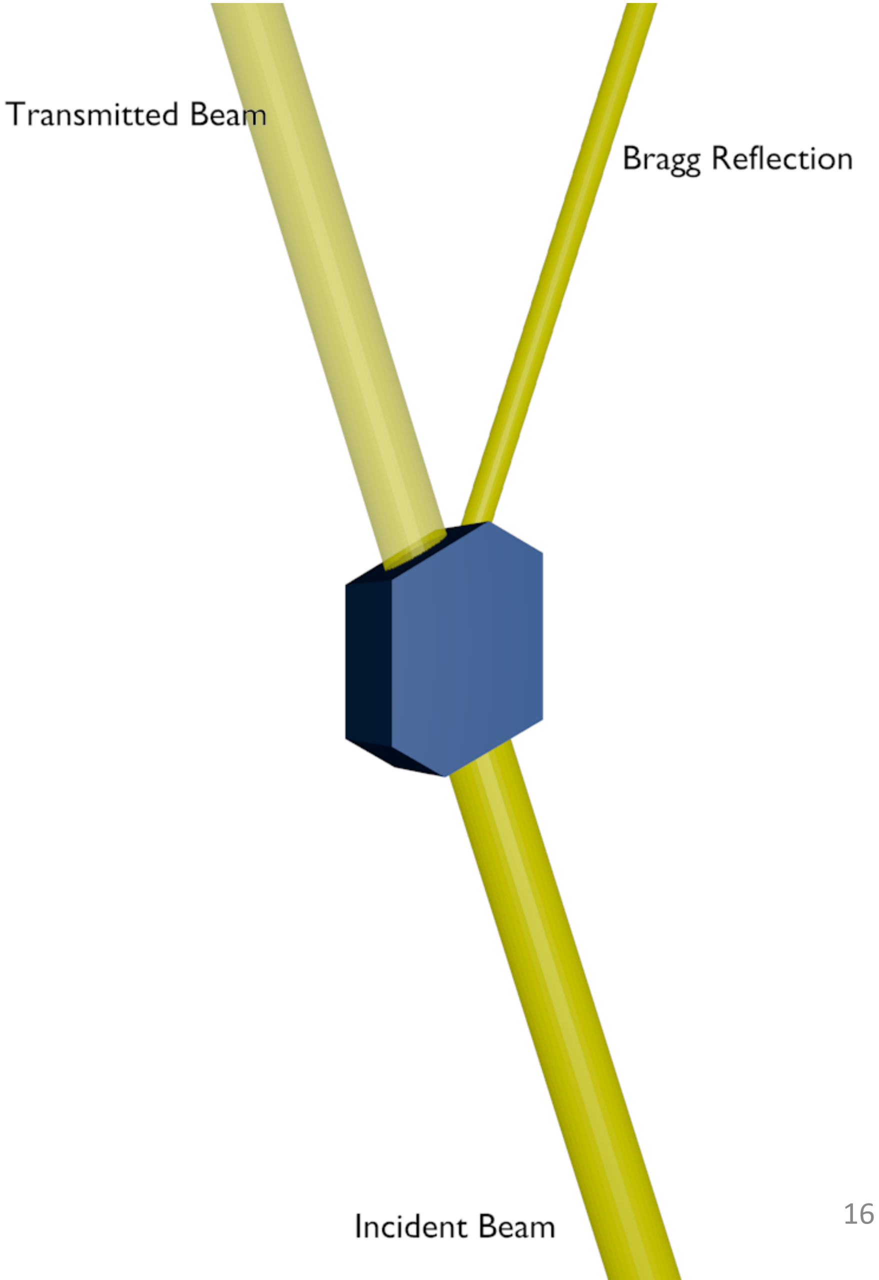
The Ewald sphere and scattering triangle

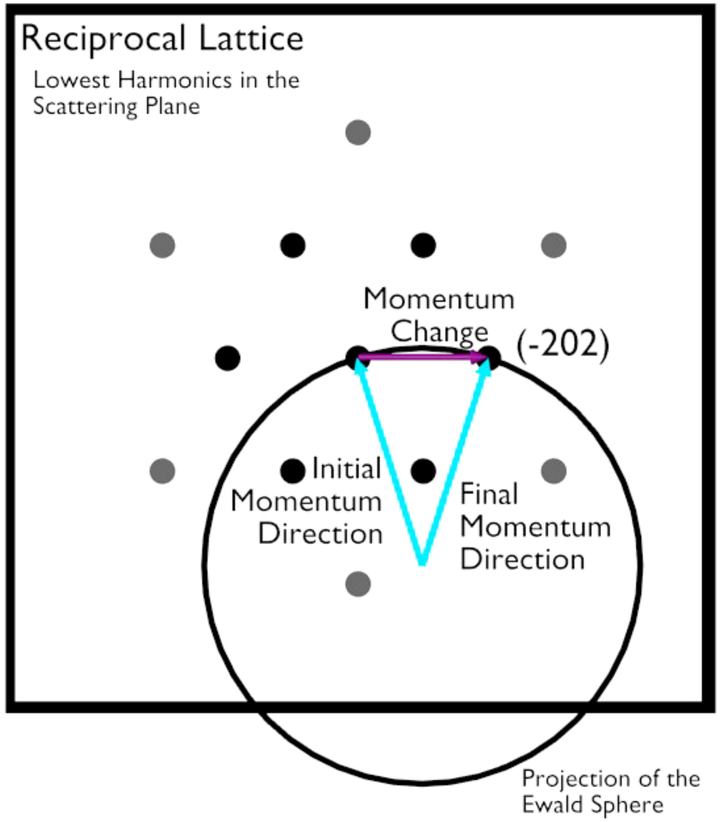


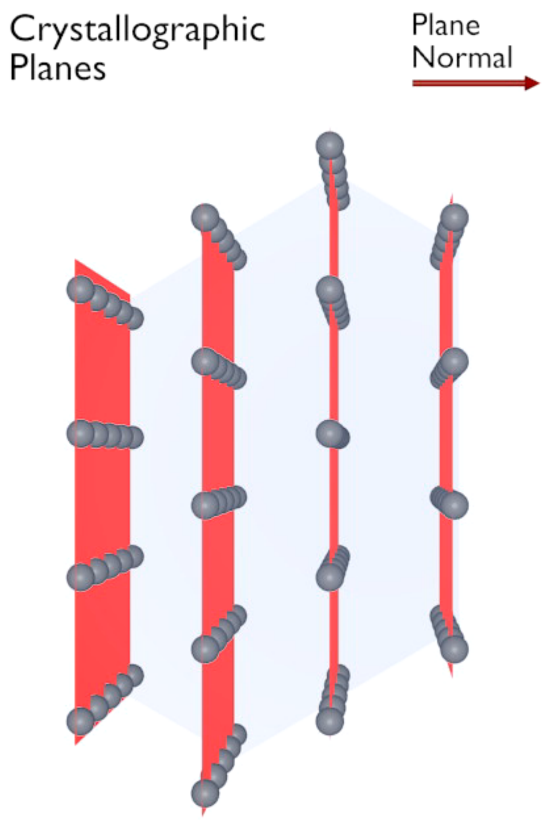


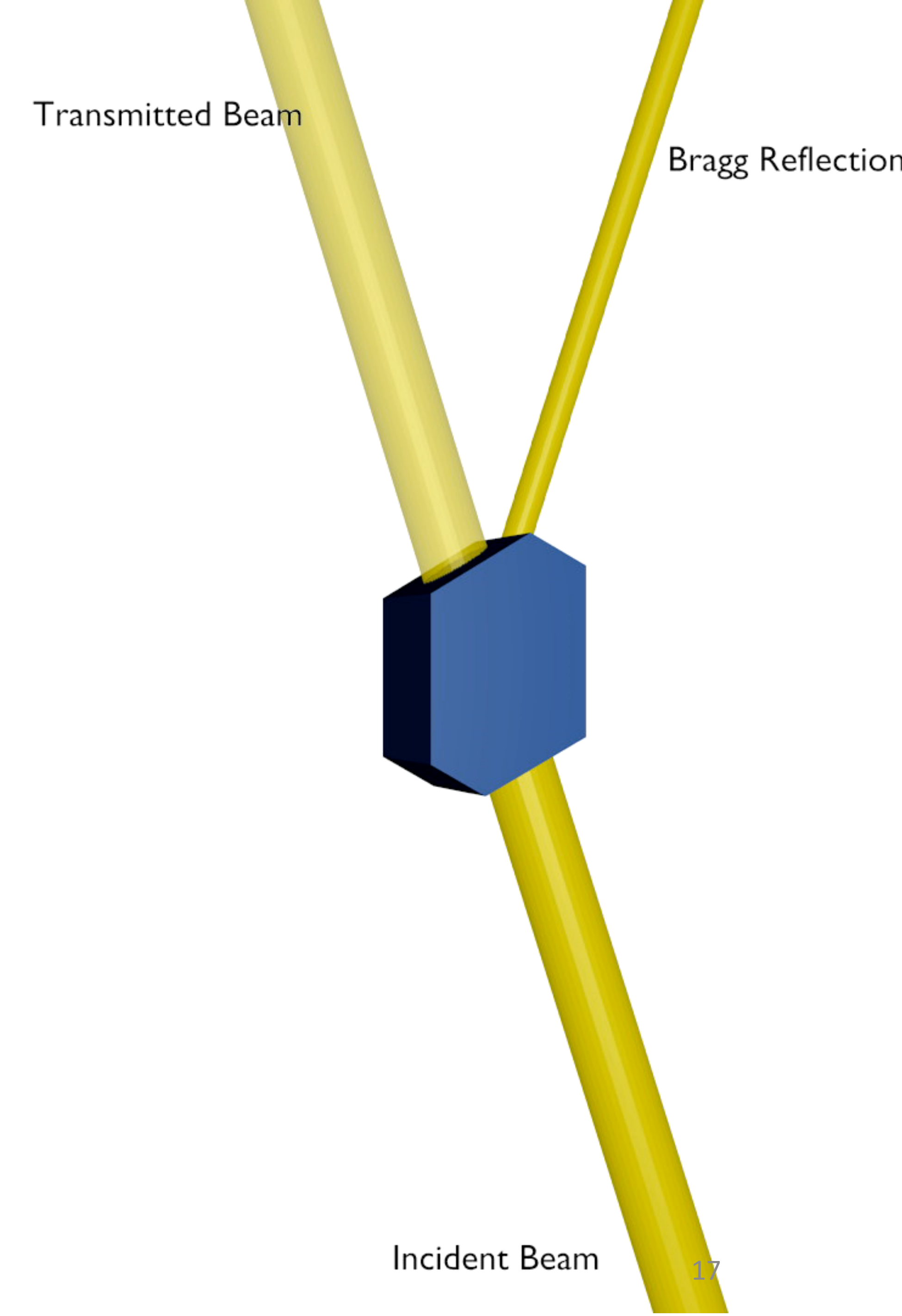
The Ewald Sphere

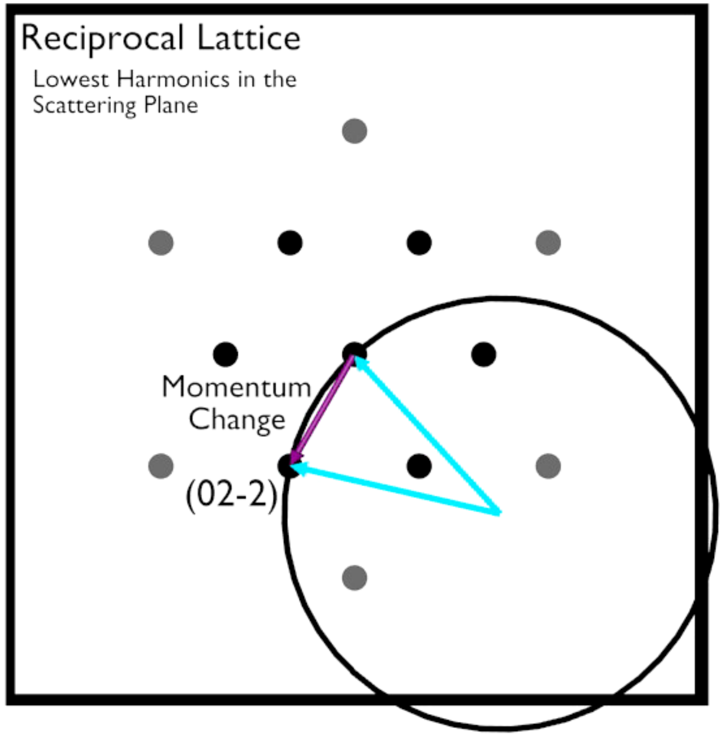
Radius is $2\pi/\lambda$

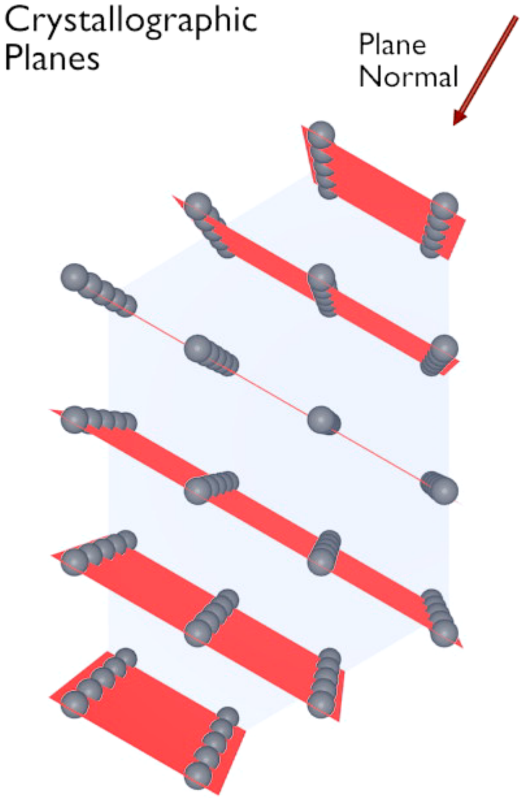



Reciprocal Lattice
Lowest Harmonics in the Scattering Plane
Momentum Change
(-202)
Initial Momentum Direction
Final Momentum Direction
Projection of the Ewald Sphere


Crystallographic Planes
Plane Normal


Transmitted Beam
Bragg Reflection
Incident Beam


Reciprocal Lattice
Lowest Harmonics in the Scattering Plane
Momentum Change
(02-2)


Crystallographic Planes
Plane Normal