Analytical Methods for Materials

Lesson 15

Reciprocal Lattices and Their Roles in Diffraction Studies

Suggested Reading

Chs. 2 and 6 in Tilley, Crystals and Crystal Structures, Wiley (2006)

Ch. 6 – M. DeGraef and M.E. McHenry, Structure of Materials, Cambridge (2007).

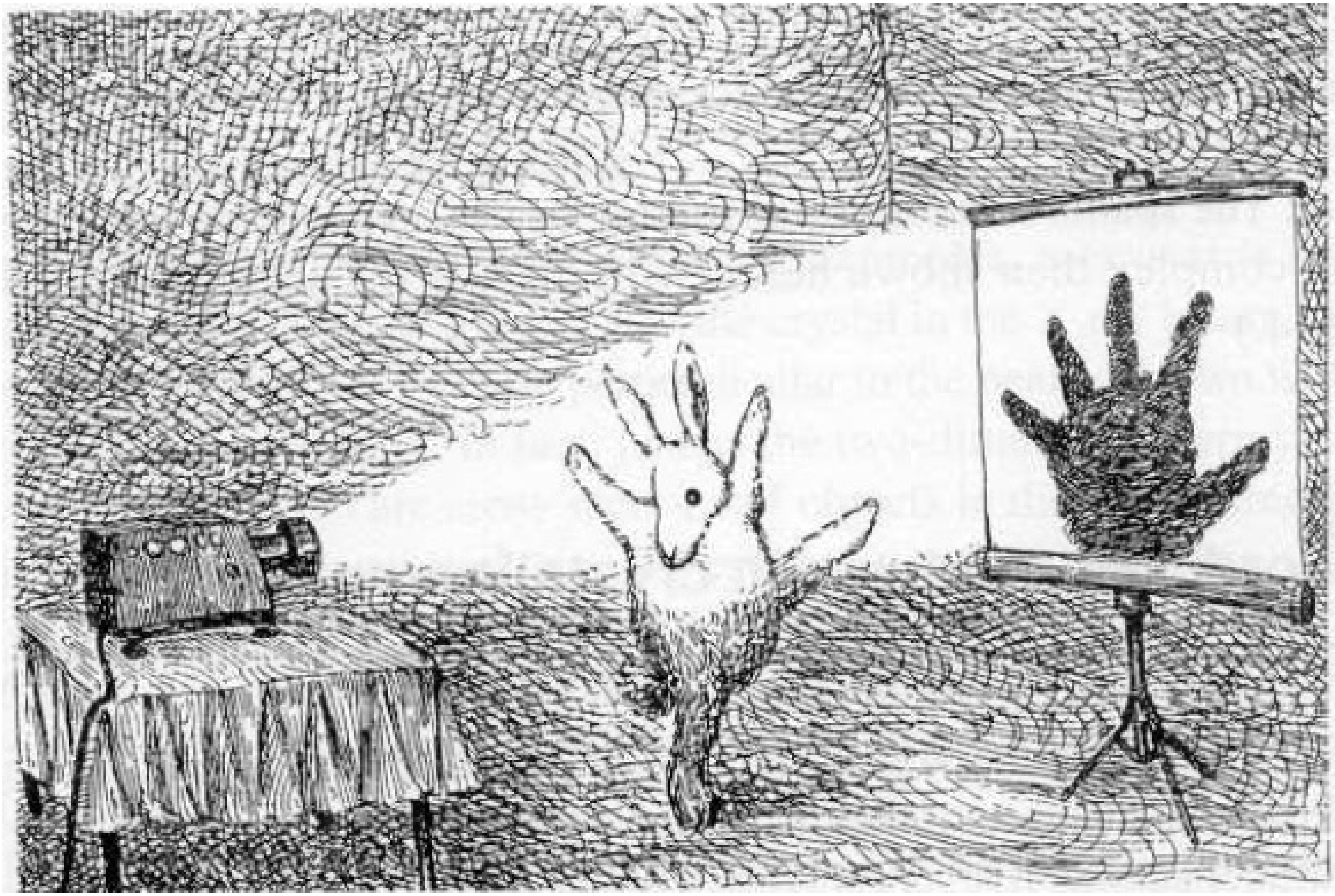
Appendix A from Cullity & Stock

Corresponding to any crystal lattice in ‘real’ space is a reciprocal lattice

Our interest stems from the fact that many properties are reciprocal to those of the crystal lattice.

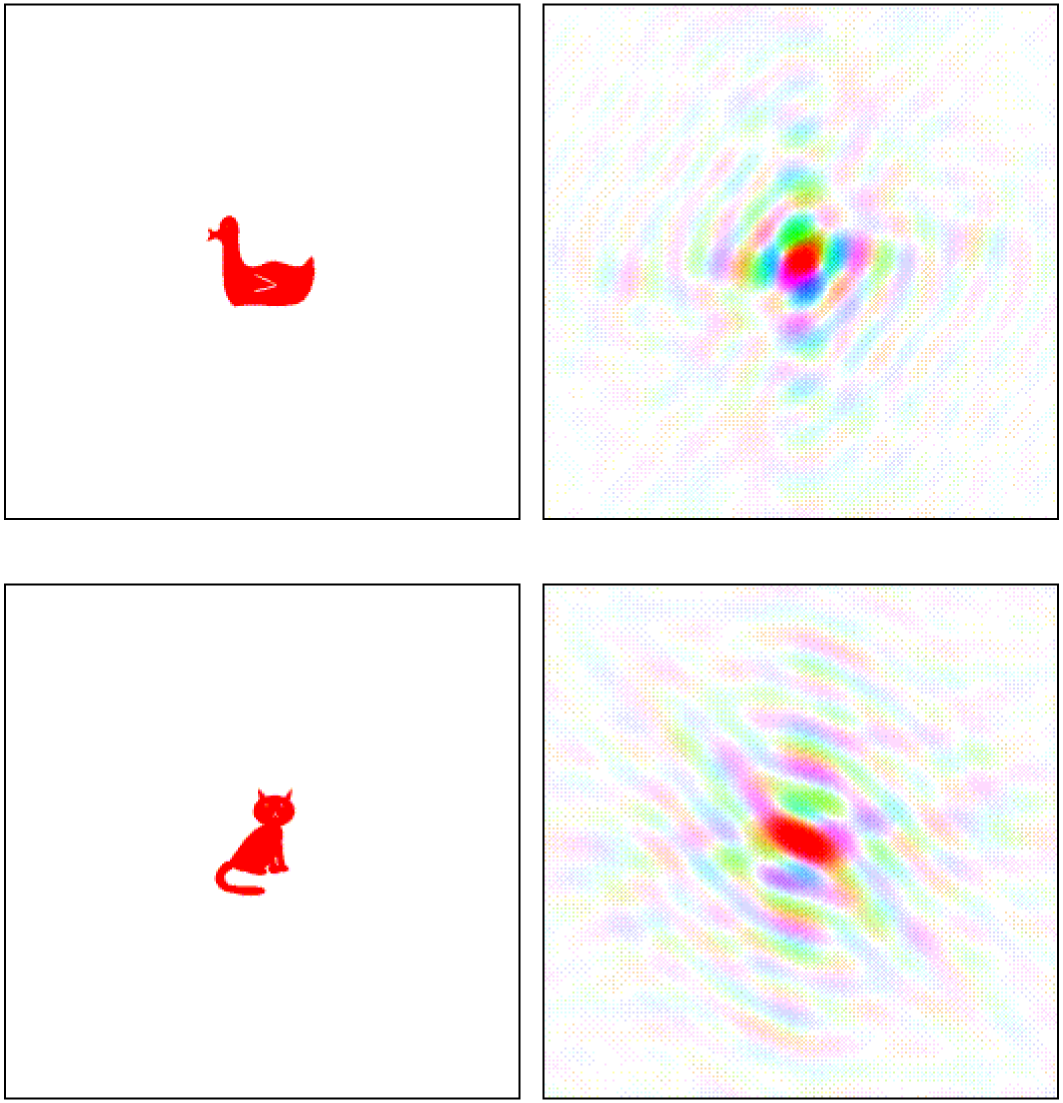
Do you remember what I said on Day 1 of the class:

crystals diffraction is inverse to lattice spacings! 



Fun in reciprocal space, © The New Yorker Collection, 1991. John O'Brien, from http://www.cartoonbank.com.

Things can look very different in reciprocal space than in real space.



Things can look very different in reciprocal space than in real space.

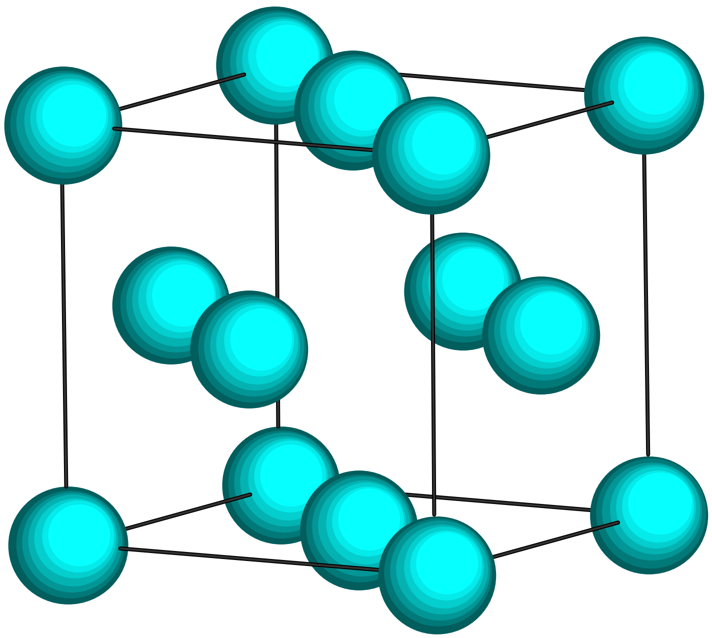
Reciprocal Lattice

- Provides a vector representation of crystal directions and spacing between diffracting planes.

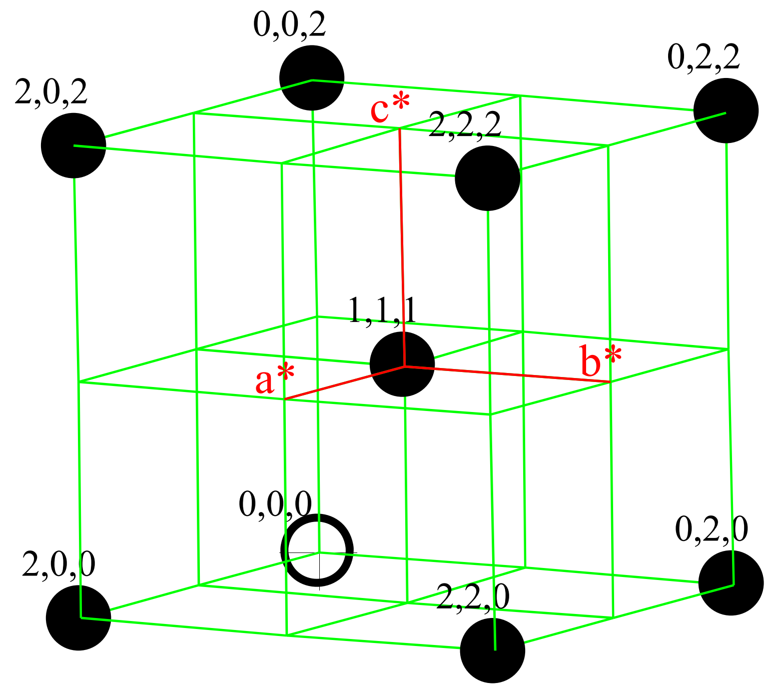
- Real Space: (lattice parameters define lattice)
  - $a, b, c, \alpha, \beta, \gamma$

- Reciprocal Space: (just another type of lattice)
  - $a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*$

FCC Crystal



Real Space

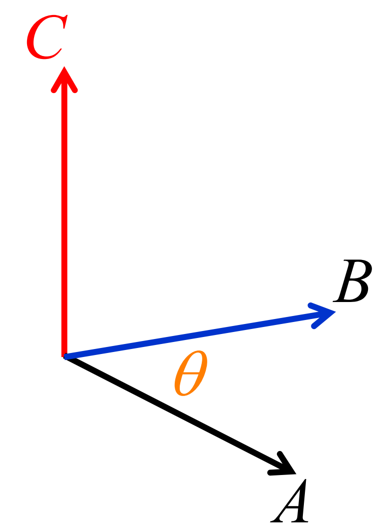


Reciprocal Space

Recall some simple vector operations

- Dot product (scalar product):

$$A \cdot B = \underset{\sqrt{h^2+k^2+l^2}}{|A|}\,\underset{\sqrt{h^2+k^2+l^2}}{|B|}\cos\theta$$



- Cross product (vector product):

$$A \times B = C = |A||B|\sin\theta$$

$$C \text{ is the direction } \perp A - B \text{ plane}$$

- Other useful relations (and there are more…)

$$A \times B = C = -(B \times A)$$

$$A \cdot (B \times C) = B \cdot (C \times A) = C \cdot (A \times B)$$

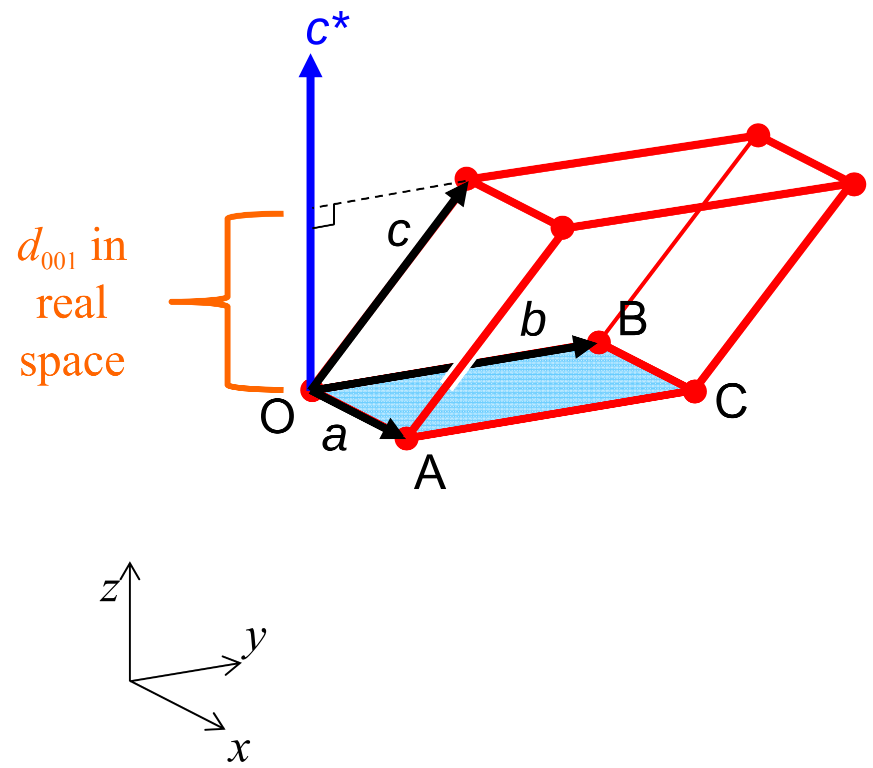
Reciprocal Vectors

$$\left|c^*\right| = \left|\frac{(a \times b)}{c \cdot (a \times b)}\right|$$

$$= \left|\frac{\text{area of base}}{\text{unit cell volume}}\right|$$

$$= \frac{1}{\text{height}}$$

$$= \frac{1}{d_{001}} = c^*$$



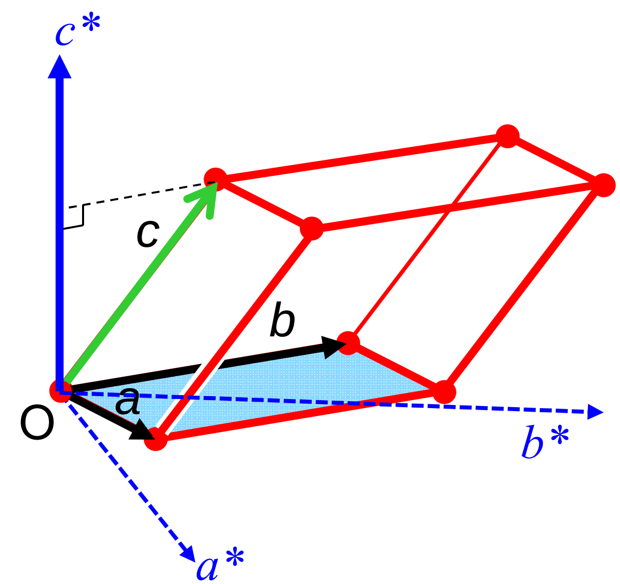
Thus, we can define entire reciprocal lattices

- For an arbitrary lattice [$a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma (\neq 90°)$] in real space.

$$a^* = \frac{(b \times c)}{a \cdot (b \times c)} = \frac{(b \times c)}{V}$$

$$b^* = \frac{(c \times a)}{b \cdot (c \times a)} = \frac{(c \times a)}{V}$$

$$c^* = \frac{(a \times b)}{c \cdot (a \times b)} = \frac{(a \times b)}{V}$$



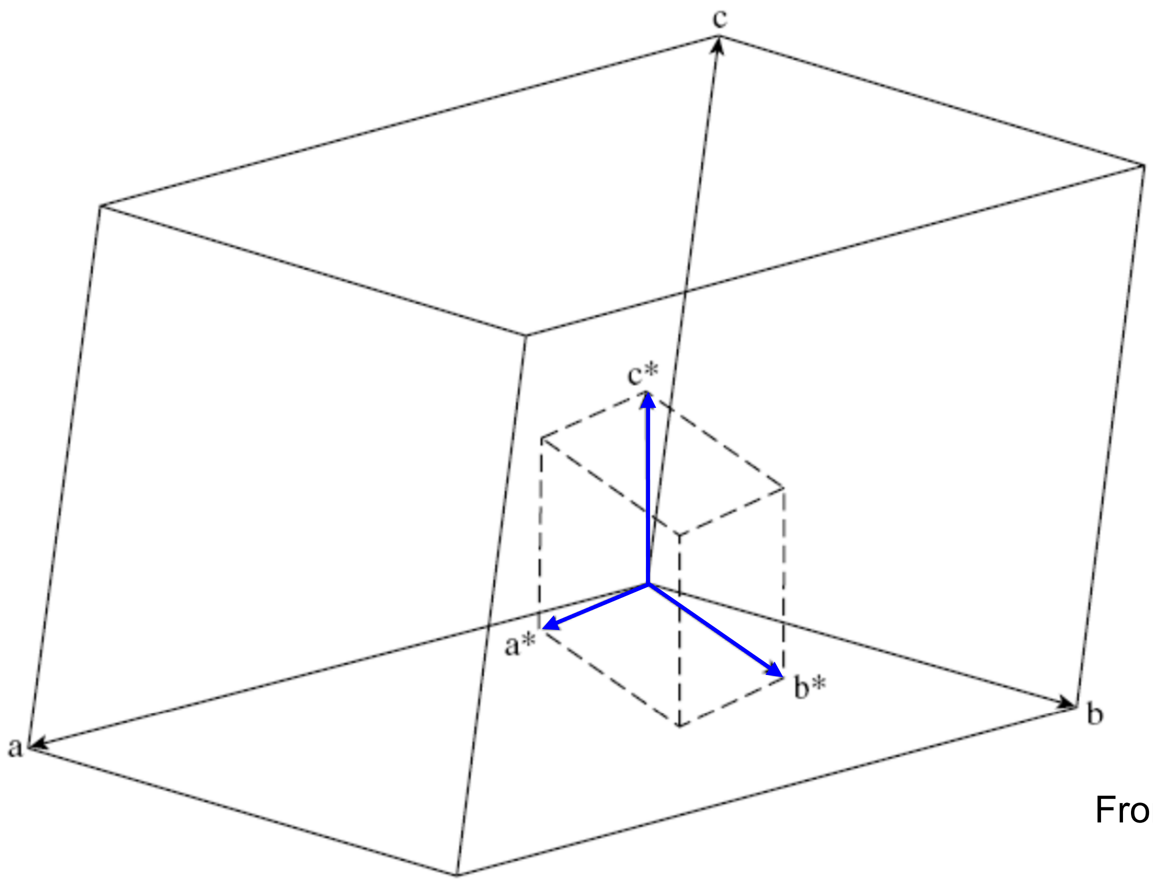
$$V \equiv \text{unit cell volume } = a \cdot (b \times c) = b \cdot (c \times a) = c \cdot (a \times b)$$

$a^* \perp bc$ plane in real space; it is the reciprocal lattice vector for a

$b^* \perp ac$ plane in real space; it is the reciprocal lattice vector for b

$c^* \perp ab$ plane in real space; it is the reciprocal lattice vector for c

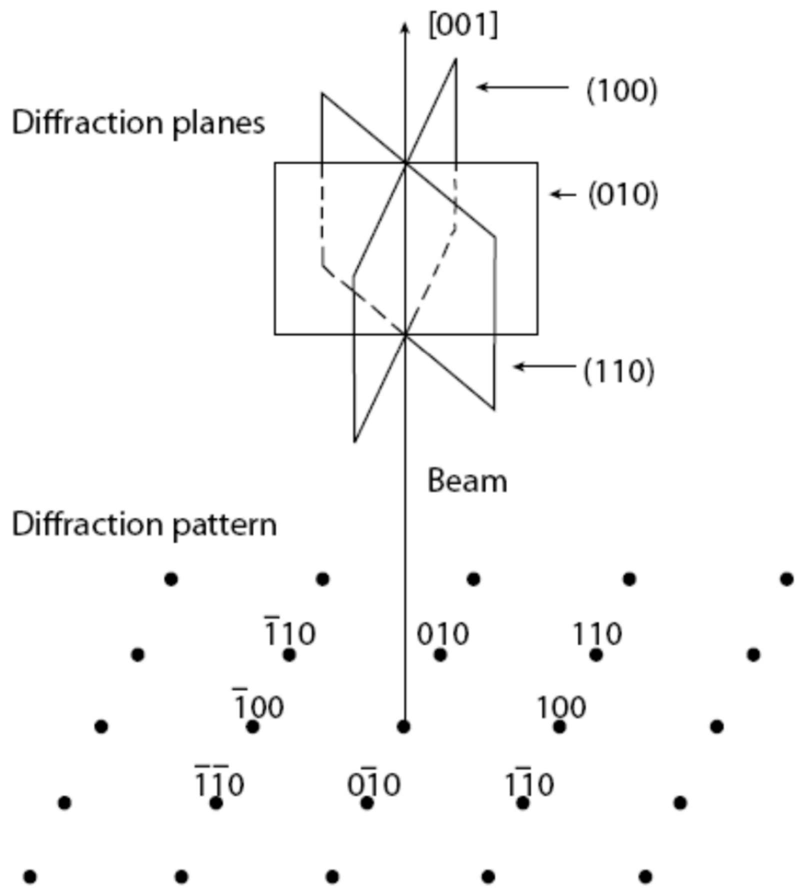
Example of the relationship between the real lattice and the reciprocal lattice.



From Leng, p. 52

Figure 2.8 Relationship between directions of unit vectors in a real crystal lattice (**a**, **b**, **c**) and its reciprocal lattice (**a***, **b***, **c***). **a*** must be perpendicular to **b** and **c** because **a*** is perpendicular to the (100) plane. Generally, **a*** is not parallel to **a** except in orthogonal systems.

Example of the relationship between the real lattice and the reciprocal lattice.



From Leng, p. 53

Figure 2.9 Relationship between a reciprocal lattice plane and real space directions. The reciprocal lattice plane is composed of diffraction spots from crystal planes (hk0). The zone axis [001] is perpendicular to the reciprocal lattice plane.

Useful Properties of the reciprocal lattice

$$\left|a^*\right| = \frac{1}{d_{100}} = a^*$$

$$\left|b^*\right| = \frac{1}{d_{010}} = b^*$$

$$\left|c^*\right| = \frac{1}{d_{001}} = c^*$$

$$\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$$

$$\cos\beta^* = \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\gamma\sin\alpha}$$

$$\cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

Relationship between real and reciprocal

In orthogonal real lattices
($a = b = c$ and $\alpha = \beta = \gamma (= 90°)$)

$$a^* \perp a;\ b^* \perp b;\ c^* \perp c$$

Not necessarily so in non-orthogonal lattices

We can draw an analogy between reciprocal and real lattices:

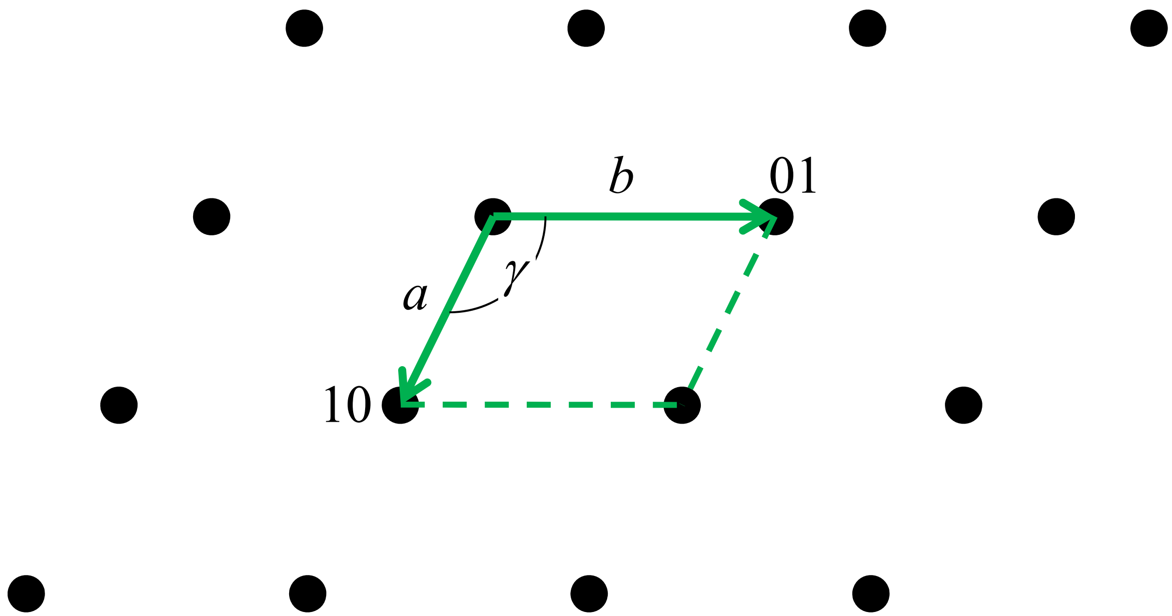
$$r_{uvw} = ua + vb + wc$$

We use this to build a real lattice from unit cells

$$r^*_{hkl} = ha^* + kb^* + lc^*$$

We can use this principle to build a reciprocal lattice

Construction of a 2D reciprocal lattice



(a) draw the plane lattice and mark the unit cell

Adapted from R. Tilley, *Crystals and Crystal Structures*,
John Wiley & Sons, Hoboken, NJ, 2006

Construction of a 2D reciprocal lattice

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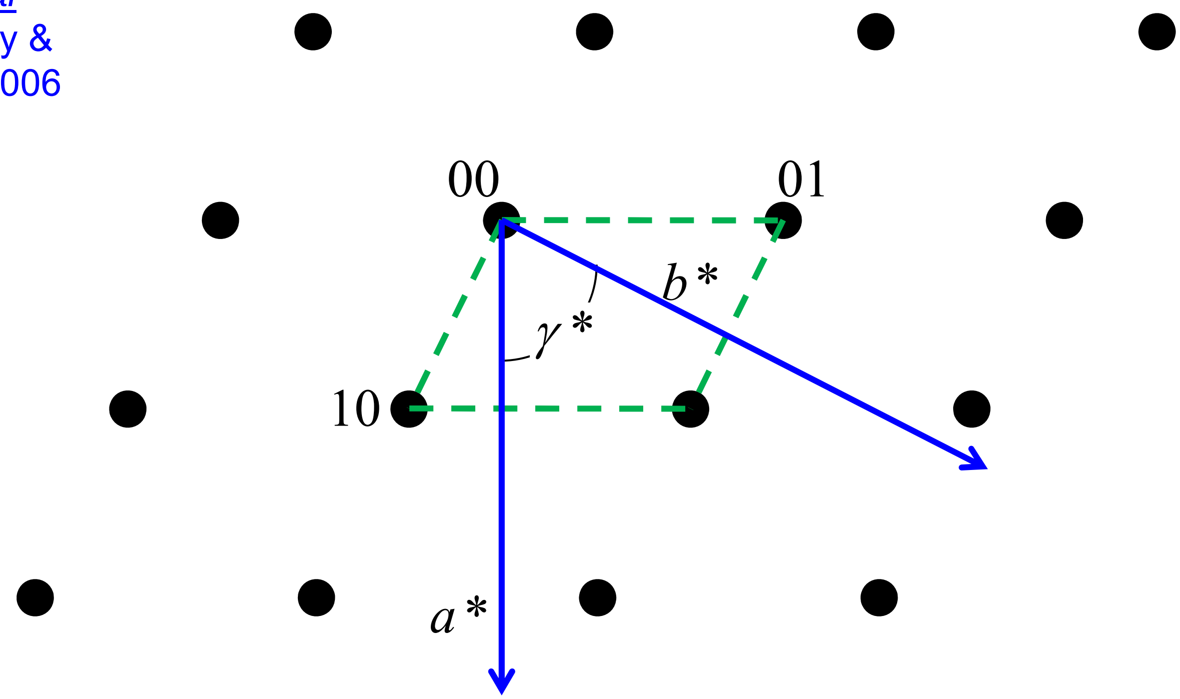
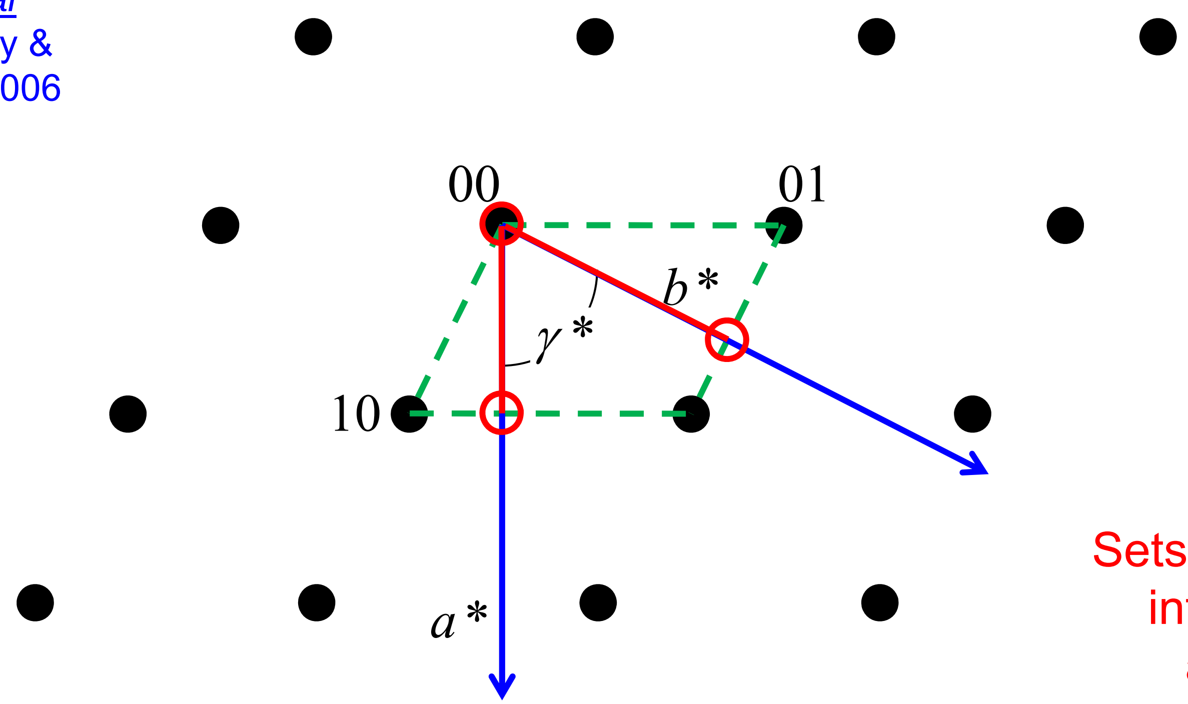


(b) draw lines perpendicular to the two sides of the unit cell to give the axial directions of the reciprocal lattice basis vectors.

Construction of a 2D reciprocal lattice

Adapted from R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006



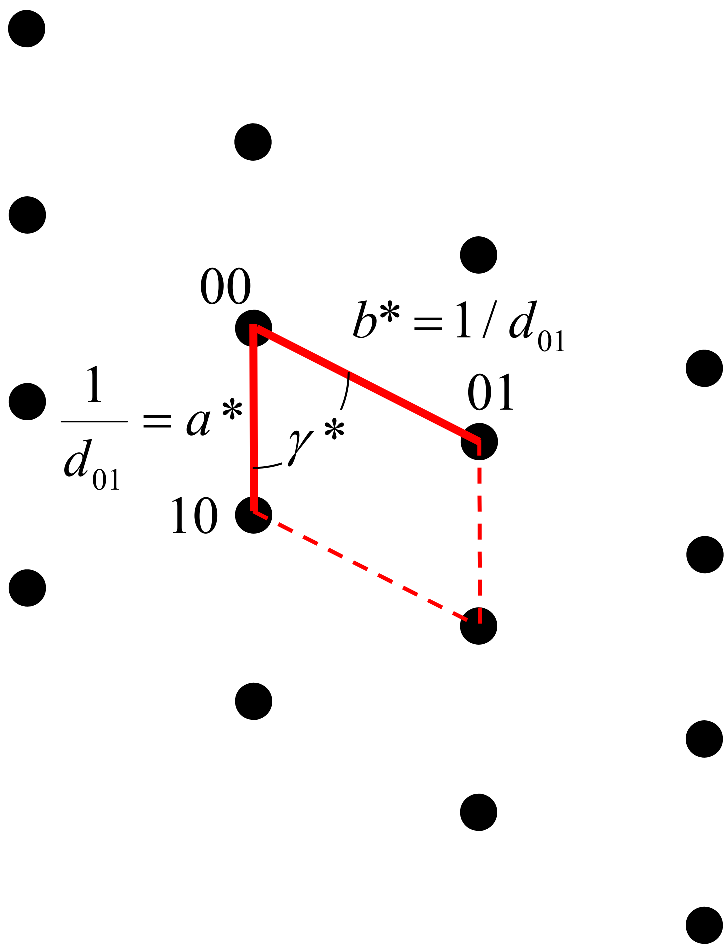
Sets axes and interaxial angle

What you're doing first is finding the spacing between the planes making up the unit cell sides.

(c) determine the perpendicular distances from the origin of the direct lattice to the end faces of the unit cell, d_{10} and d_{01}, and take the inverse of these distances, $1/d_{10}$ and $1/d_{01}$, as the reciprocal lattice axial lengths, a^* and b.

Construction of a 2D reciprocal lattice

Adapted from R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006



Draw reciprocal lattice using axes
a* **= 1/*d*$_{10}$**
b* **= 1/*d*$_{01}$**

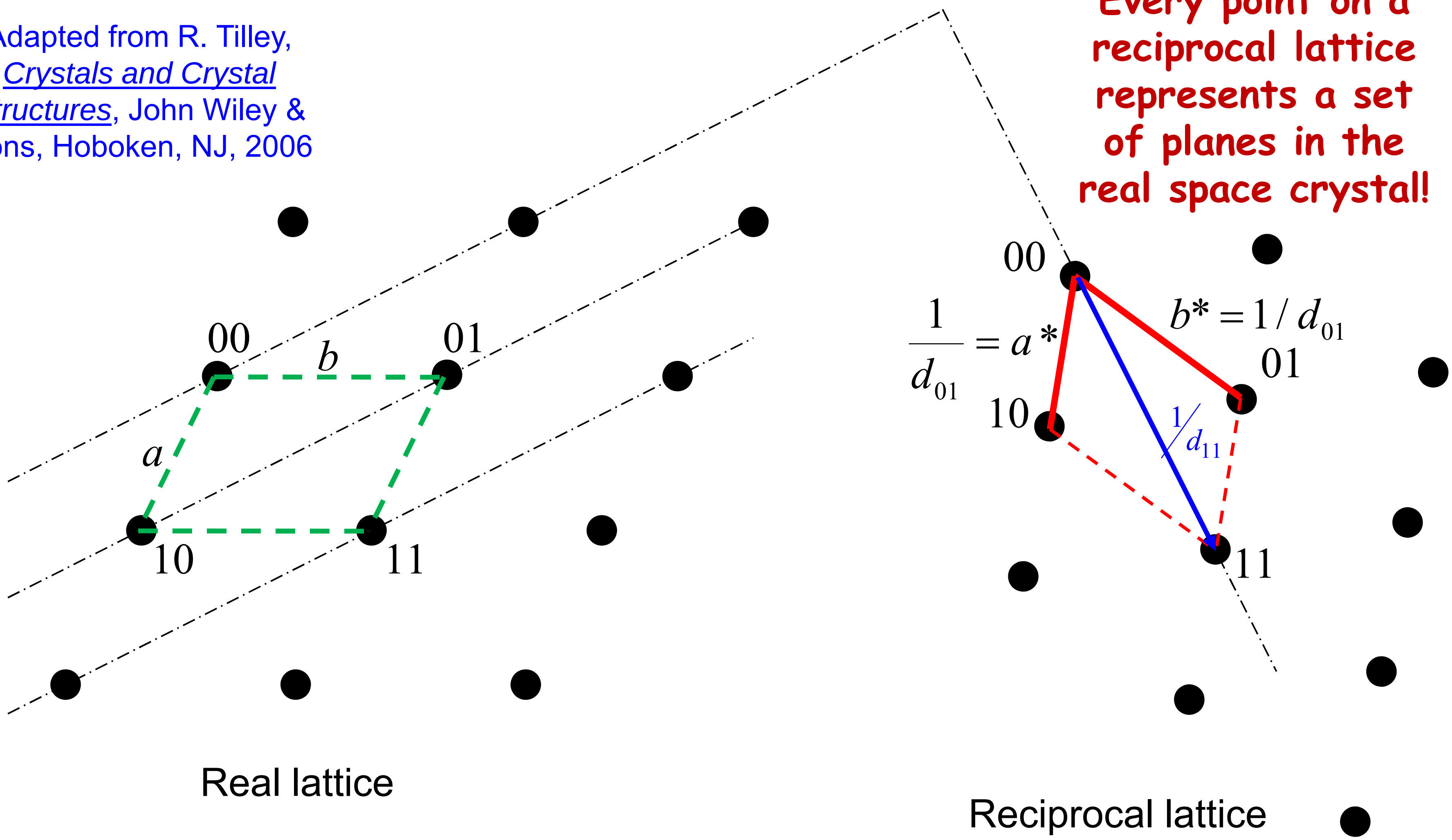
Take reciprocals to get reciprocal lattice parameters.

(d) mark the lattice points at the appropriate reciprocal distances, and complete the lattice.

Construction of a 2D reciprocal lattice

Adapted from R. Tilley, _Crystals and Crystal Structures_, John Wiley & Sons, Hoboken, NJ, 2006

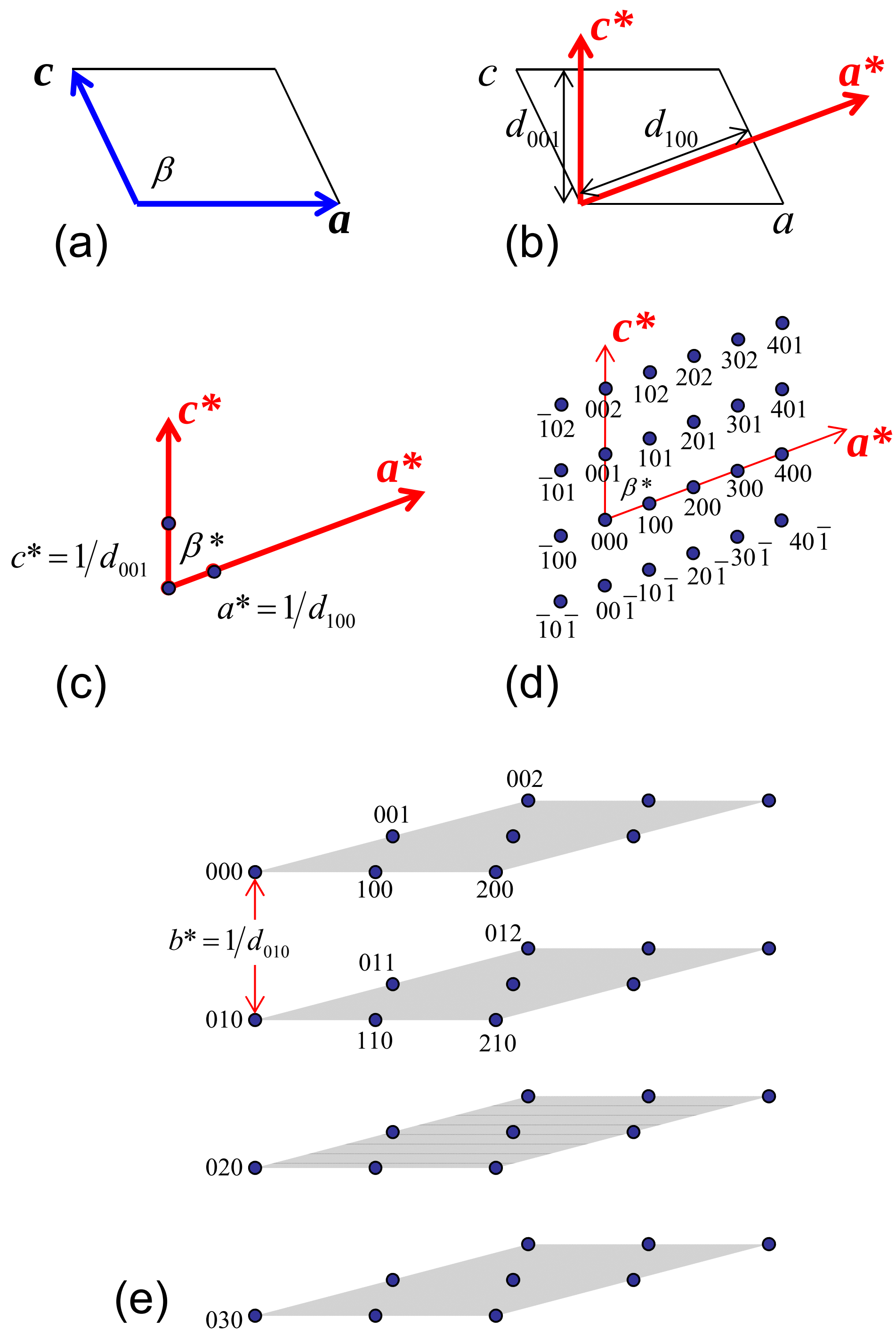
Every point on a reciprocal lattice represents a set of planes in the real space crystal!



Real lattice

Reciprocal lattice

The vector joining the origin of the reciprocal lattice to a lattice point hk is perpendicular to the (hk) planes in the real lattice and of length $1/d_{hk}$.



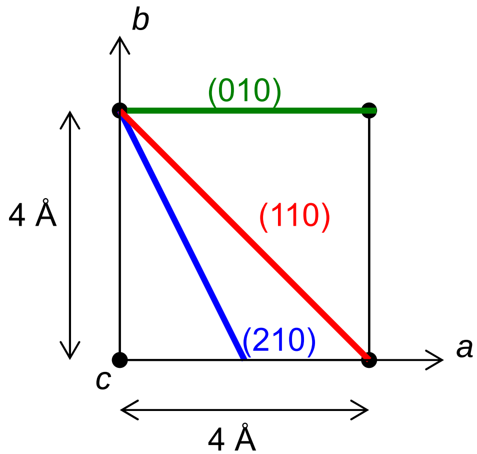
Construction of a 3D reciprocal lattice

Figure 2.10 The construction of a reciprocal lattice: (a) the **a-c** section of the unit cell in a monoclinic (*mP*) direct lattice; (b) reciprocal lattice aces lie perpendicular to the end faces of the direct cell; (c) reciprocal lattice points are spaced $a^* = 1/d_{100}$ and $c^* = 1/d_{001}$; (d) the lattice plane is completed by extending the lattice; (e) the reciprocal lattice is completed by adding layers above and below the first plane.

Adapted from R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006

Just like 2-D

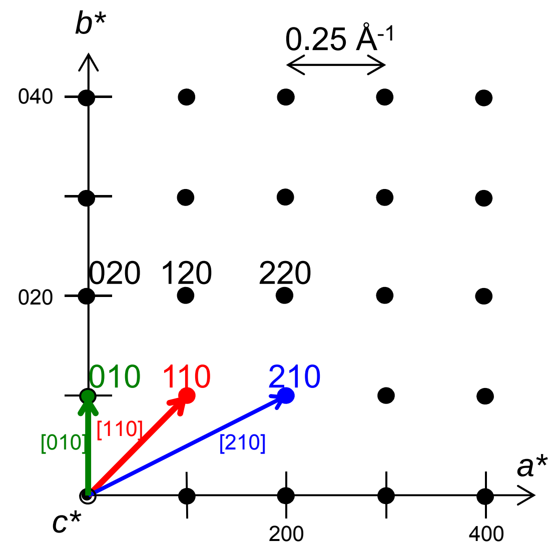
Cubic Reciprocal Lattice



REAL LATTICE

$$r_{uvw} = ua + vb + wc$$

90°

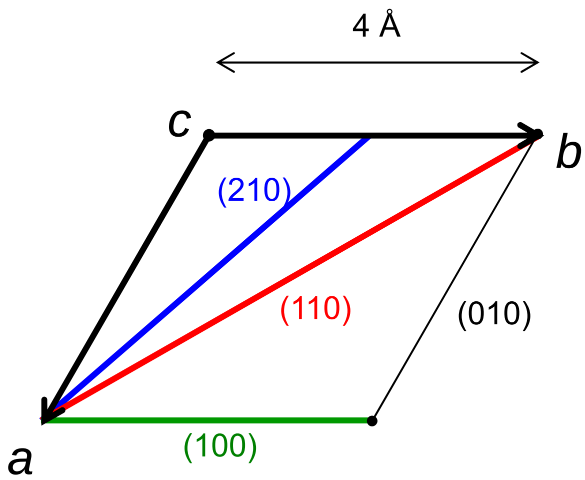


RECIPROCAL LATTICE

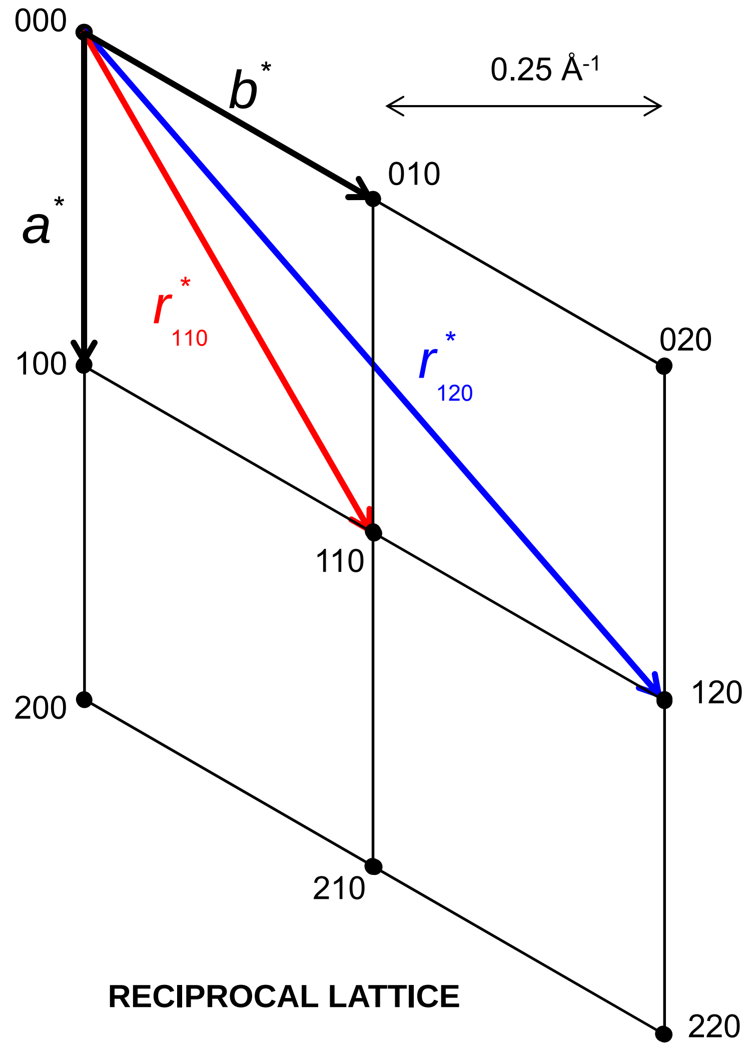
$$r^*_{hkl} = ha^* + kb^* + lc^*$$

- Every point on a reciprocal lattice represents a set of planes in the real space crystal!
- Reciprocal lattice vectors are 90° away from realspace planes!

Hexagonal Reciprocal Lattice



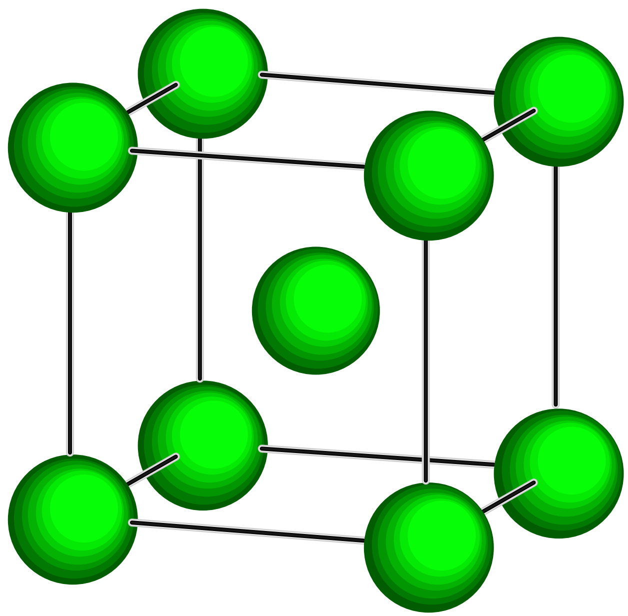
NORMAL LATTICE



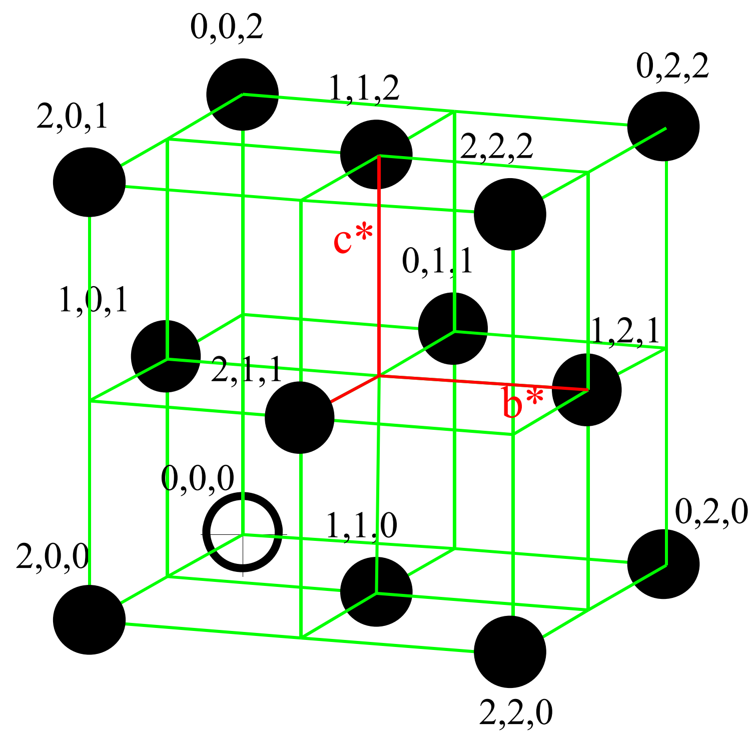
RECIPROCAL LATTICE

- Every point on a reciprocal lattice represents a set of planes in the real space crystal!

What does the BCC reciprocal lattice look like?



Real Space



Reciprocal Space

Importance of Reciprocal Space

- When a diffraction event occurs, the diffracted waves/pattern will “match” the reciprocal lattice.

★ • REASON:

EM radiation scatters in inverse proportion to the spacing between diffraction centers (i.e., planes in crystals).

Why use reciprocal space

- Bragg's Law: **(Defines conditions where a crystal is oriented for coherent scattering)**

$$n\lambda = 2d\sin\theta$$

We can combine n and d as follows:

$$d_{hkl} = \frac{d}{n}$$

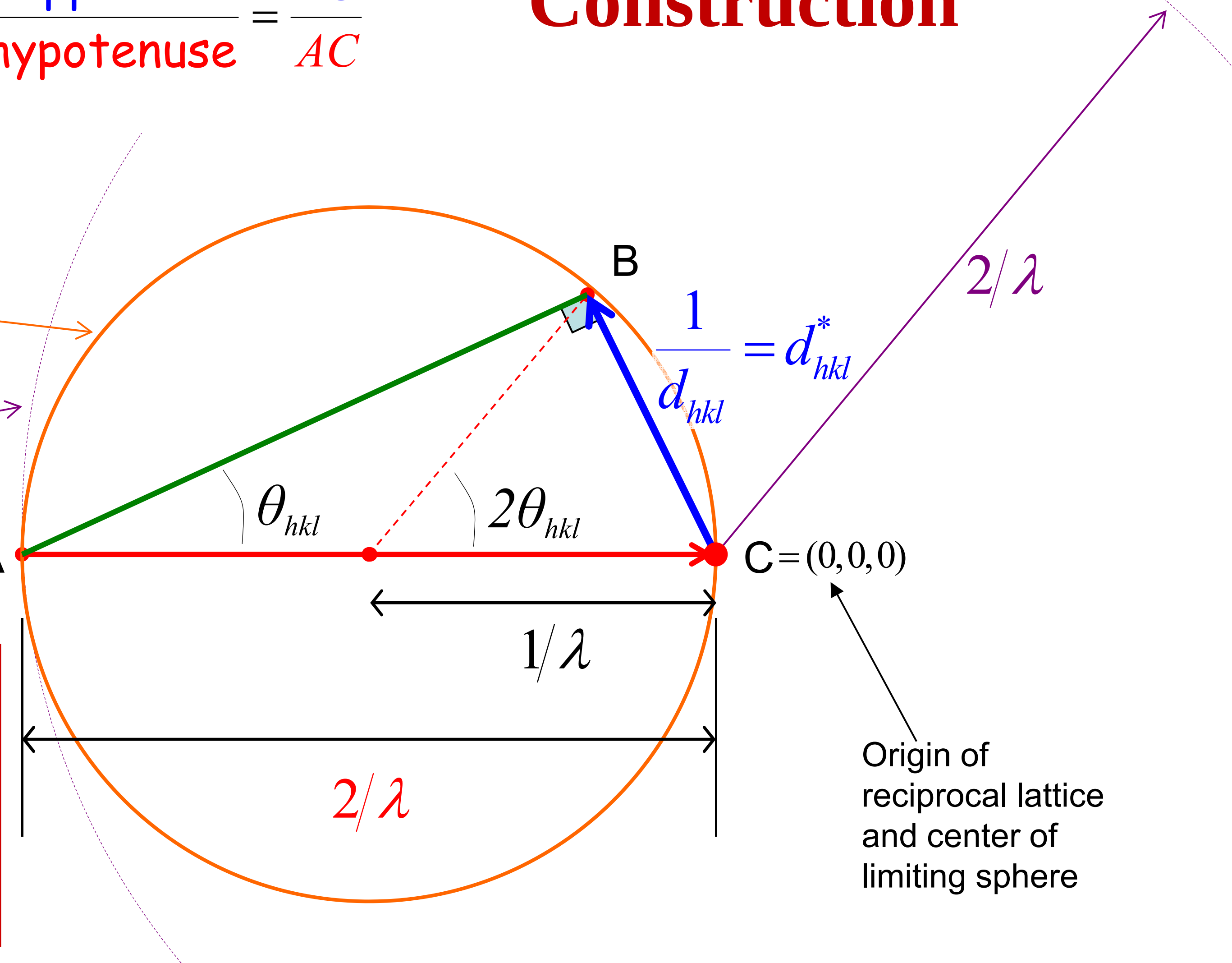
This allows us to write Bragg's Law as:

$$\lambda = 2d_{hkl}\sin\theta_{hkl}$$

$$\sin\theta_{hkl} = \frac{\lambda/2}{d_{hkl}} = \frac{\frac{1}{d_{hkl}}}{\frac{2}{\lambda}} = \frac{\text{opposite}}{\text{hypotenuse}}$$

Ewald Sphere Construction

$$\sin\theta_{hkl} = \frac{\lambda/2}{d_{hkl}} = \frac{\frac{1}{d_{hkl}}}{\frac{2}{\lambda}} = \frac{\text{opposite}}{\text{hypotenuse}} = \frac{BC}{AC}$$



CRITICAL

Only lattice points lying within the limiting sphere can diffract. Points lying on the Ewald sphere will satisfy the Bragg condition.

See this web site for an explanation and example
http://www.msm.cam.ac.uk/doitpoms/tlplib/xray-diffraction/ewald.php

$$\sin\theta = \frac{OB}{CO} = \frac{OB}{2/\lambda}$$

Which can be re-written as:

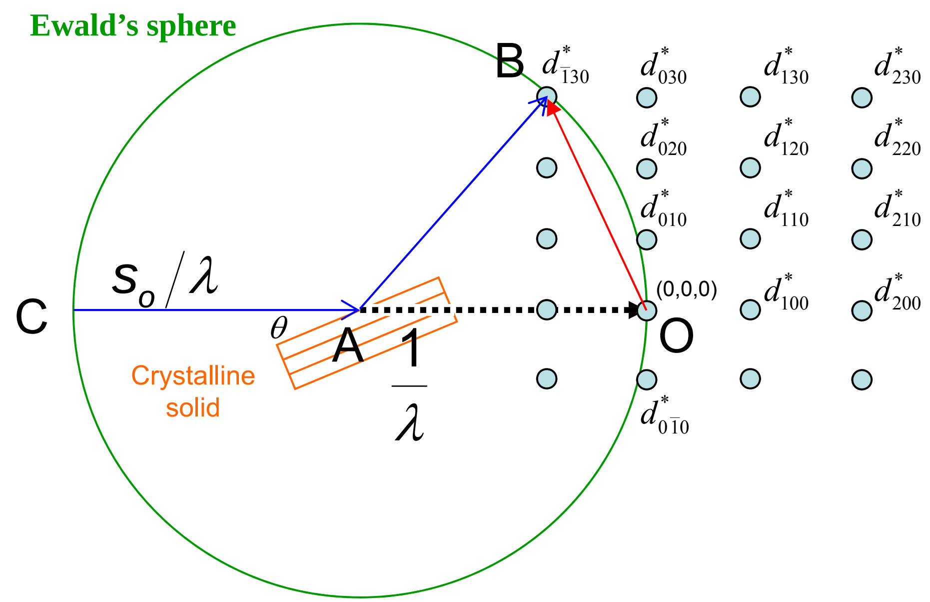
$$2\frac{1}{OB}\sin\theta = \lambda$$

Since *B* is a reciprocal lattice point:

$$OB = \frac{1}{d_{hkl}} = d^*_{hkl} = g$$

$$\therefore \frac{1}{OB} = d_{hkl} \text{ and } 2d_{hkl}\sin\theta = \lambda$$

[Bragg's Law]



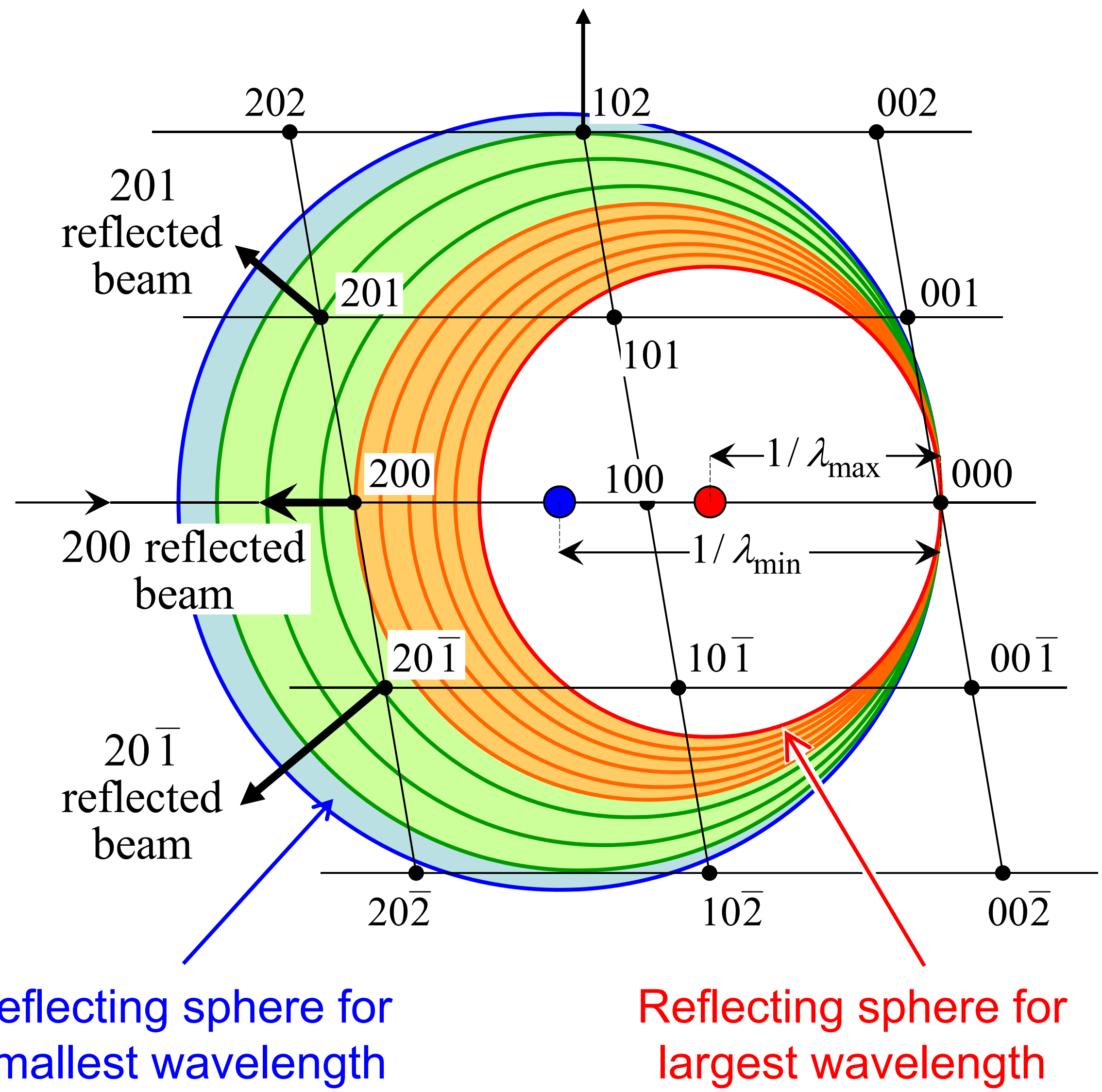
RECIPROCAL SPACE

- Size of sphere corresponds to wavelength of radiation used (see next page).
- Rotation of the crystal will cause points to lie on the sphere.
- When points lie on the sphere, Bragg's law is satisfied!

If you change λ, you change the radius of the Ewald's sphere.

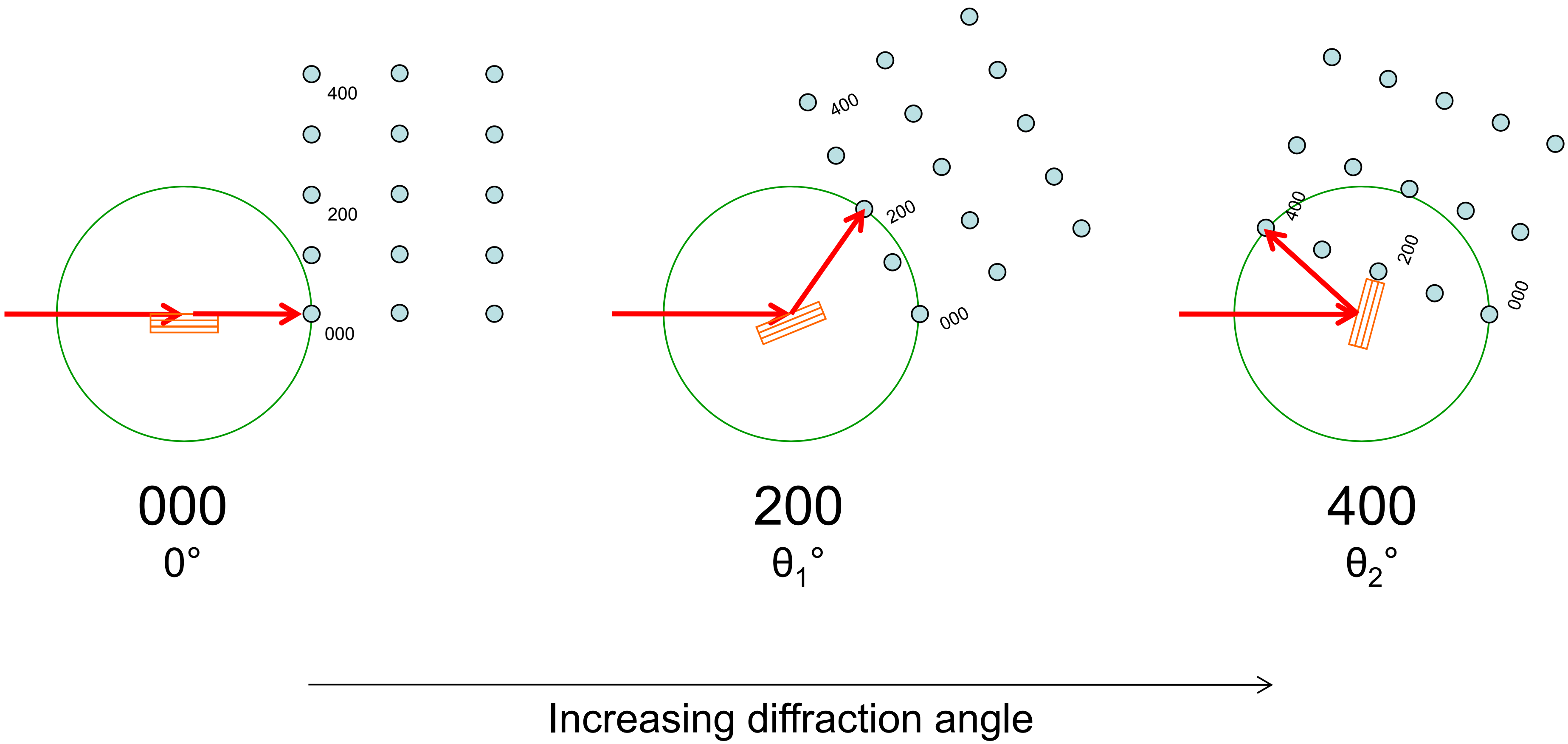
This is how the Laue technique works.

Diffractometers generally use fixed λ and variable θ.



Adapted from C. Hammond, *The Basics of Crystallography and Diffraction, 3rd Edition* (Oxford University Press, Oxford, UK, 2009) p. 201.

Adapted from A.D. Krawitz,
Introduction to Diffraction in Materials Science and Engineering,
Wiley, New York, 2001



Diffractometers generally use fixed λ and variable θ.

Synopsis

1. The reciprocal lattice allows us to compute the spacing between successive lattice planes in a crystal lattice.

2. The reciprocal lattice vector d^*_{hkl} with components (hkl) is perpendicular to the plane with Miller indices (hkl).

3. The length of the reciprocal lattice vector is equal to the inverse of the spacing between the corresponding planes.

4. Diffraction of X-rays (and electrons) is described by the Bragg equation, which relates the radiation wavelength (λ) to the diffraction angle (θ) and the spacing between crystal planes (d_{hkl}).