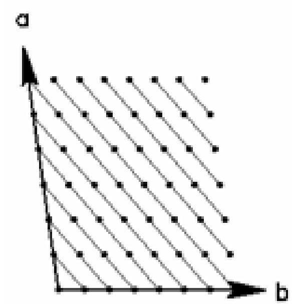
Lesson 7

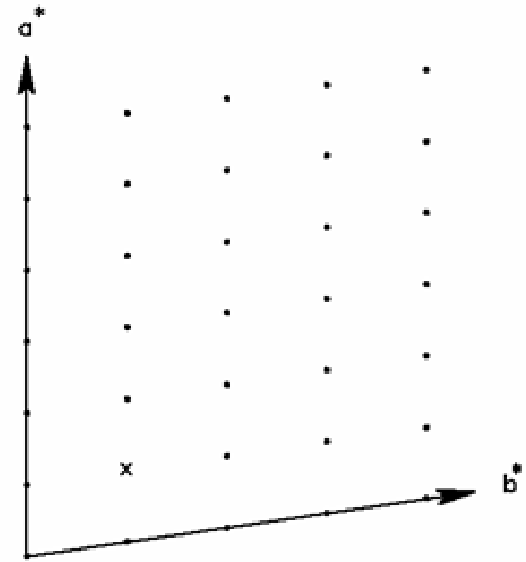
- The reciprocal cell
  - What is it?
  - How does it relate to the real cell?
  - What can we do with it
- How to put crystals into the correct position to diffract.
- This lesson deals with matters that are contained in any diffraction equipment.
- Need to “talk the talk”

How does the Reciprocal Relate to the Real Cell

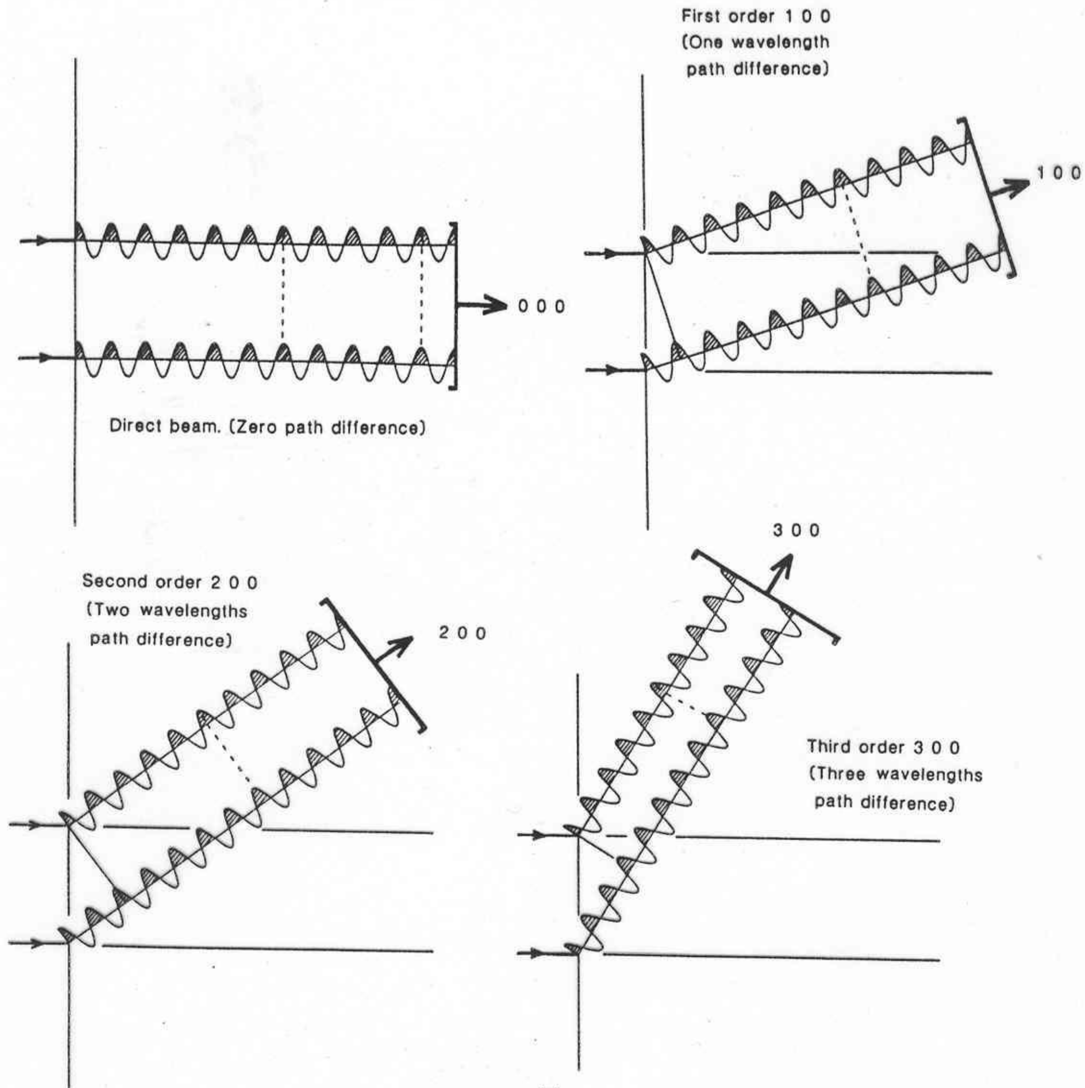
- By definition
  - **a·a*** = 1 **a·b*** = 0 **a·c*** = 0
  - **b·b*** = 1 **b·c*** = 0 **c·c*** = 1
- This means **a*** is perpendicular to the **bc** face
  b* is perpendicular to the **ac** face and
  c* is perpendicular to the **ab** face.



real space



reciprocal space


First order 1 0 0
(One wavelength
path difference)
1 0 0
0 0 0
Direct beam. (Zero path difference)
3 0 0
Second order 2 0 0
(Two wavelengths
path difference)
2 0 0
Third order 3 0 0
(Three wavelengths
path difference)

(c)

Monoclinic Cell

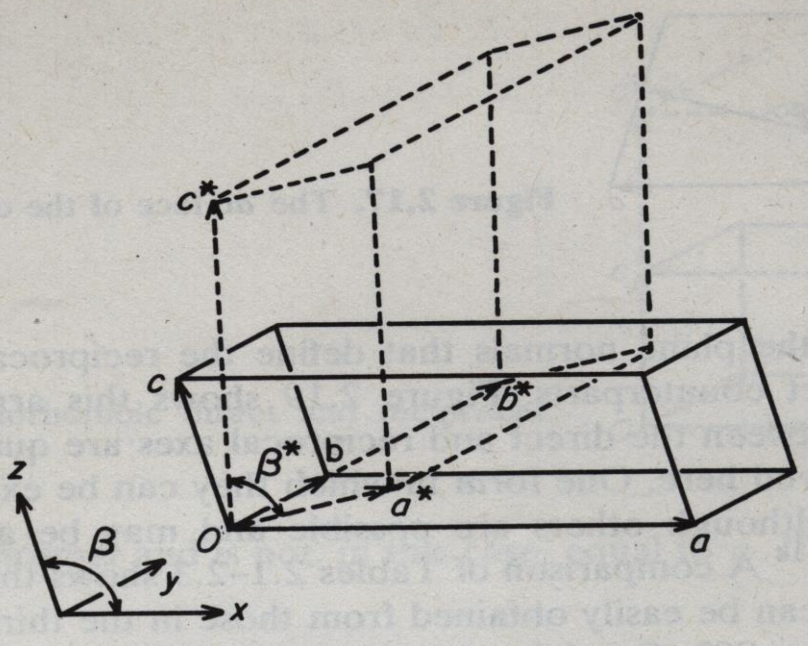


Figure 2.18. Monoclinic direct and reciprocal cells.

Triclinic Cell

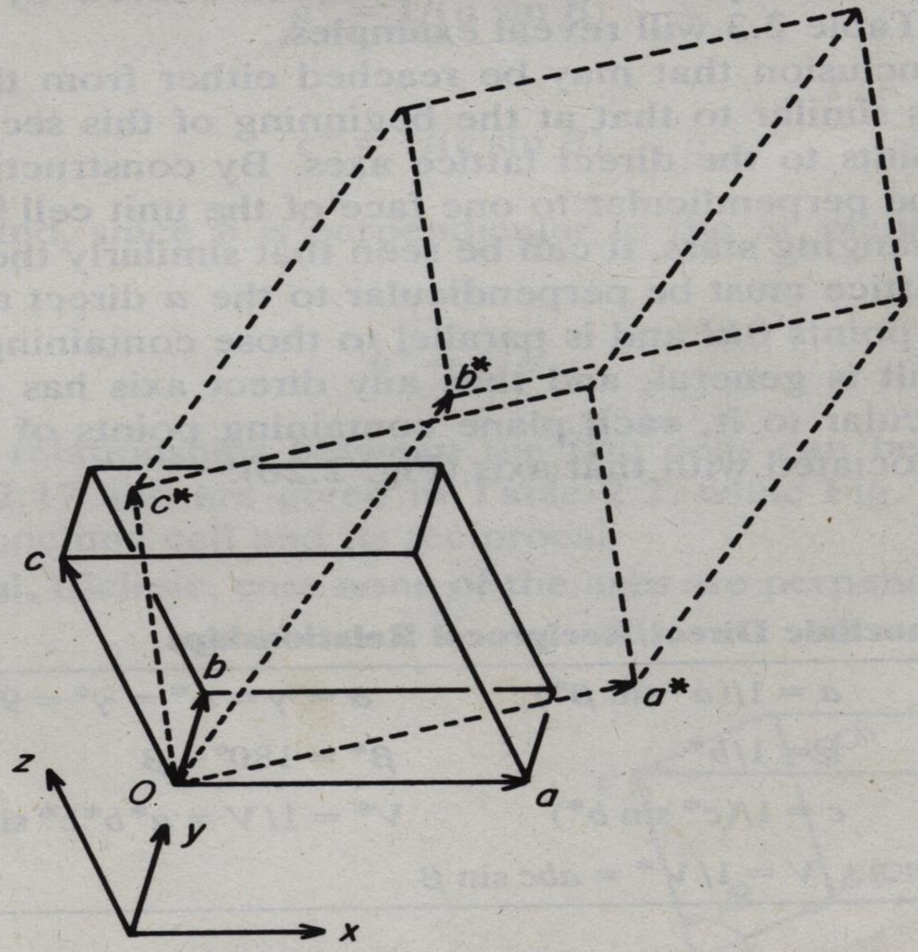


Figure 2.19. Triclinic direct and reciprocal cells.

Formulas for Conversion

TABLE 2.3 Triclinic Direct and Reciprocal Relationships

$$a^* = \frac{bc \sin \alpha}{V} \qquad a = \frac{b^* c^* \sin \alpha^*}{V^*}$$

$$b^* = \frac{ac \sin \beta}{V} \qquad b = \frac{a^* c^* \sin \beta^*}{V^*}$$

$$c^* = \frac{ab \sin \gamma}{V} \qquad c = \frac{a^* b^* \sin \gamma^*}{V^*}$$

$$V = \frac{1}{V^*} = abc\sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$$

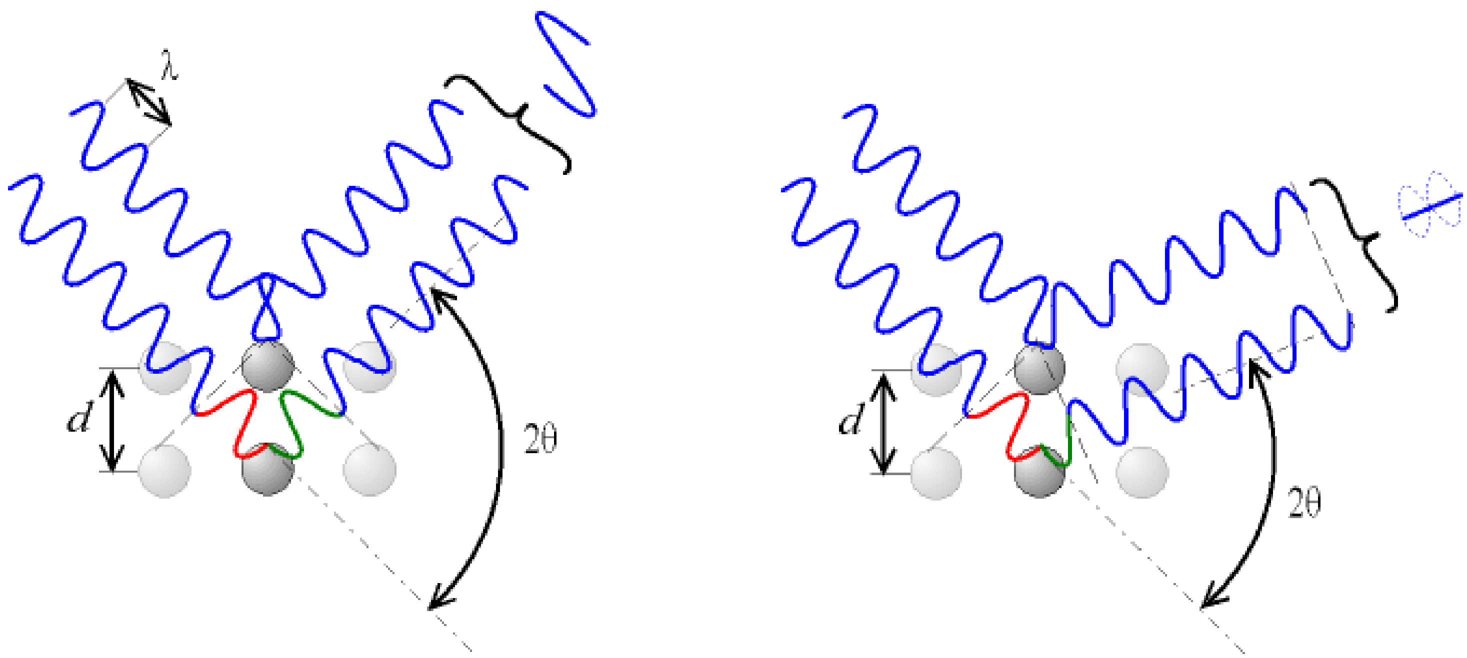
$$V^* = \frac{1}{V} = a^* b^* c^* \sqrt{1 - \cos^2 \alpha^* - \cos^2 \beta^* - \cos^2 \gamma^* + 2 \cos \alpha^* \cos \beta^* \cos \gamma^*}$$

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

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

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

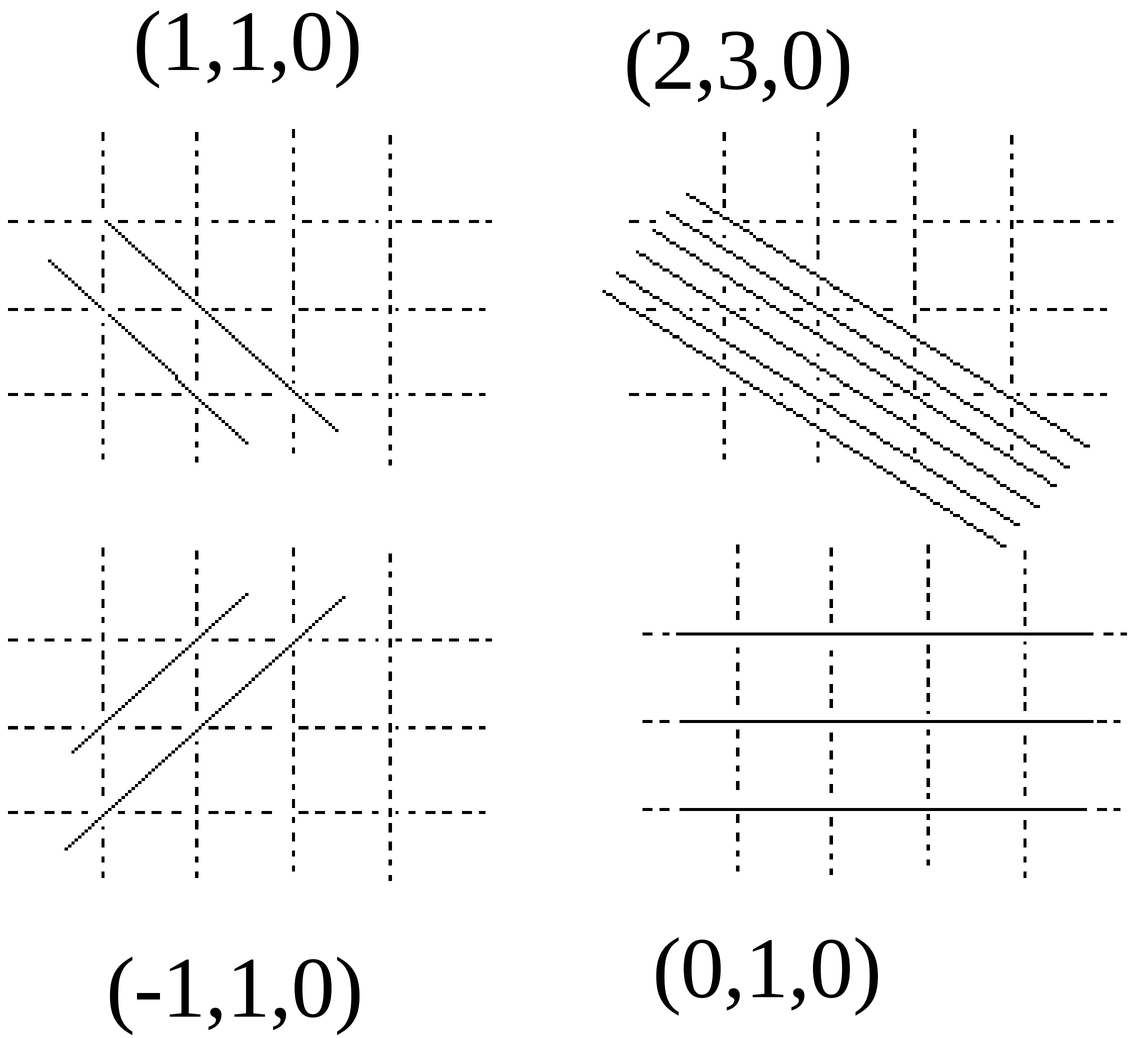
Bragg's Law

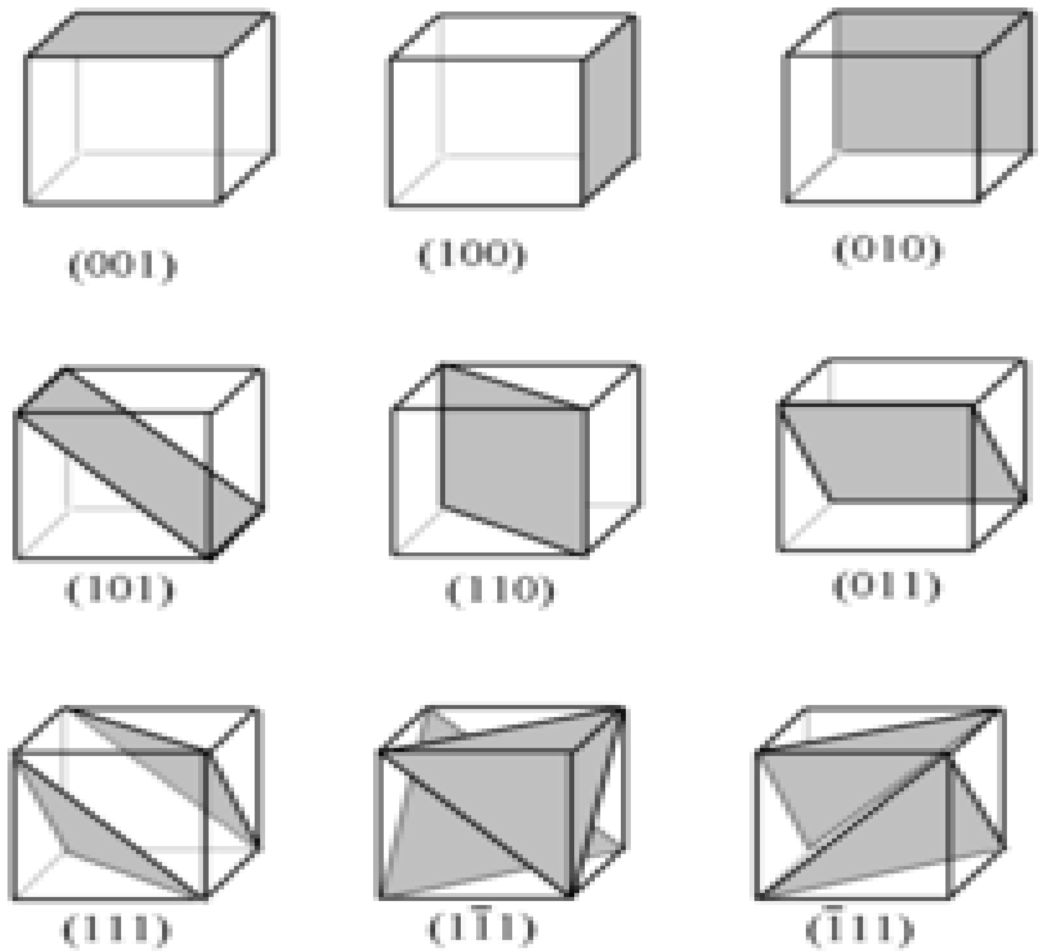


$2d\sin(\Theta)=n\lambda$

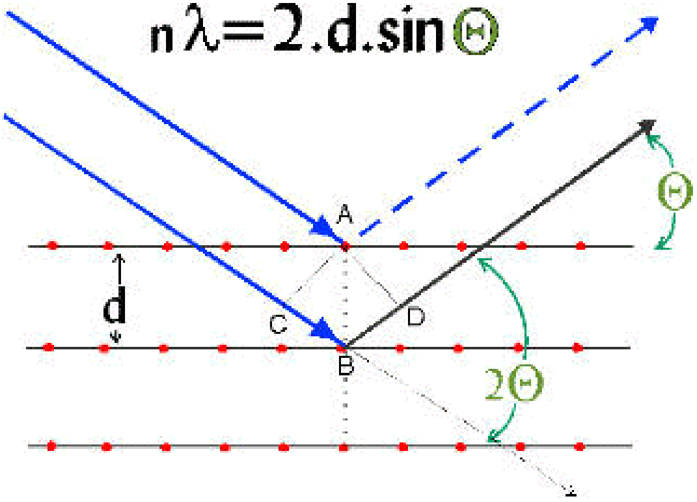
Obviously Θ can never be greater than 90°

Bragg Planes

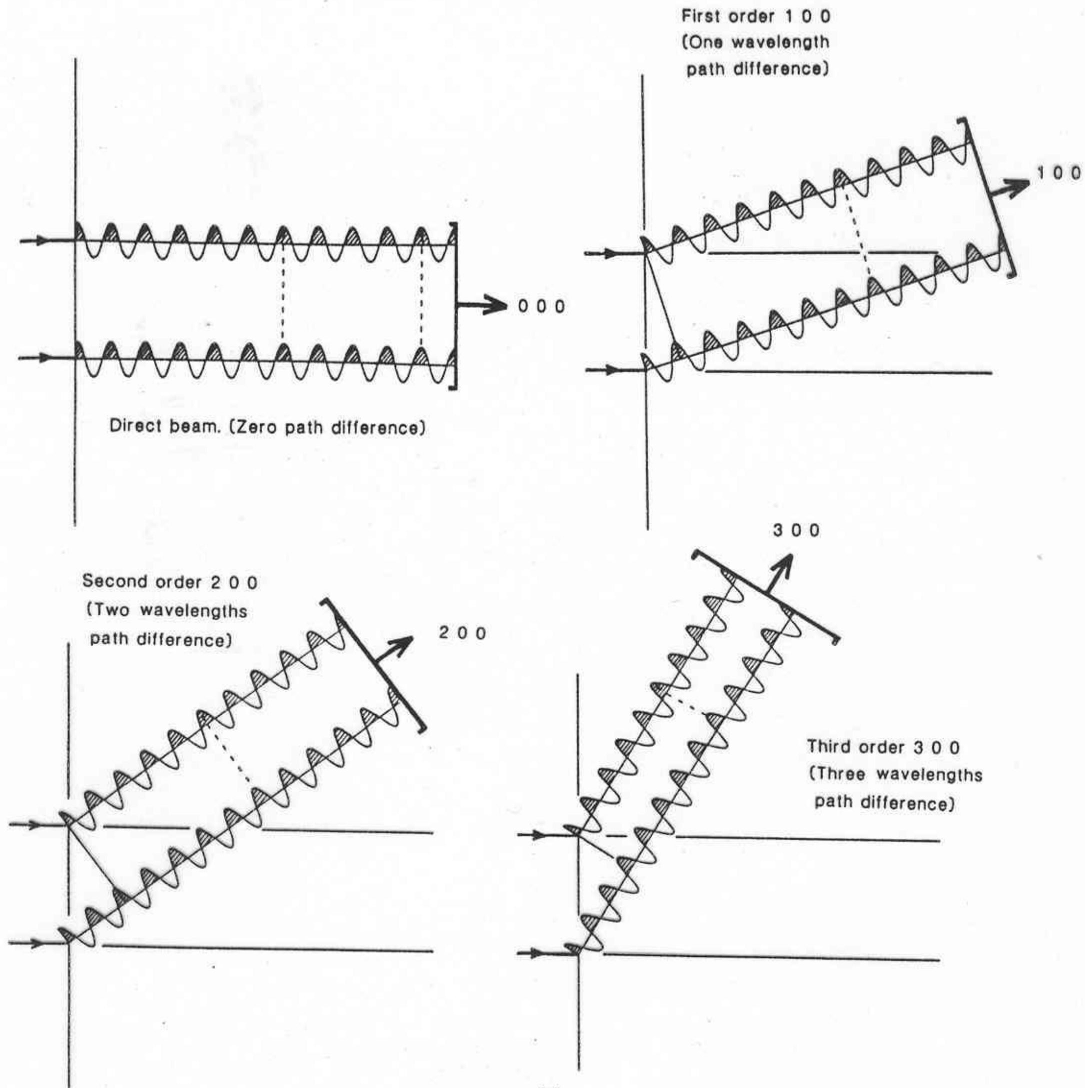



(001)
(100)
(010)
(101)
(110)
(011)
(111)
(1$\bar{1}$1)
($\bar{1}$11)

A comment on Brag Planes



The drawing implies the atoms are located on the Bragg Planes. This is usua not true. If this were the case all the atoms would have “easy” coordinates. However what is true is that the more electron denisty on a plane the greater intensity of the diffraction.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(c)

A nice feature

- The reciprocal axes are always perpendicular to the faces.
- Bragg's laws measures d for axes corresponding to vectors perpendicular to the faces.
- This means the distance d between planes is the length of the vector ha^*,kb^*,lc^*

The Reciprocal Diffraction Vector

- The reciprocal basis vectors describe a coordinate system which is always perpendicular to the Bragg planes and always has a length of 1/d the distance between the planes.
- Thus the vector (2**a***, 3**b***, 5**c***) is perpendicular to the {2,3,5} Bragg plane and its length is the distance between this family of planes.
- Call this resulting vector **d***
- Remember must use the long non-Cartesian distance formula to calculate **|d*|**

Reciprocal Lattice

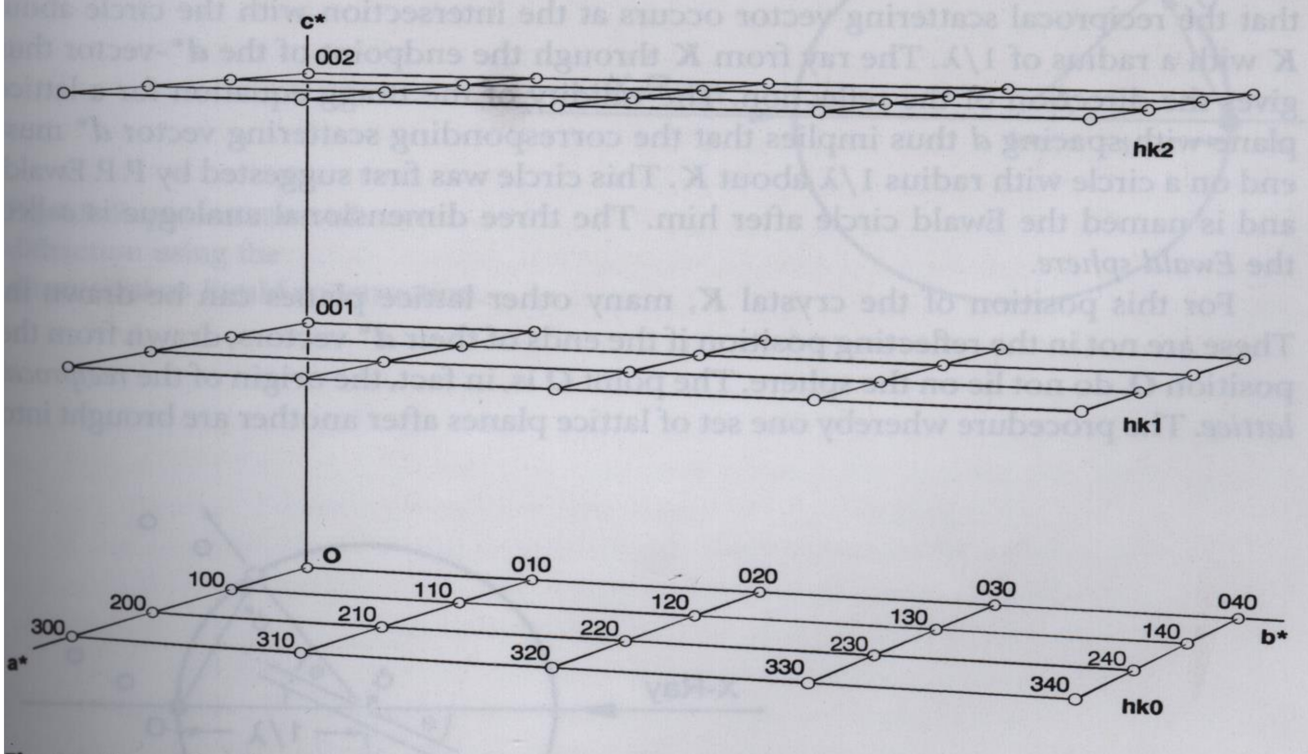
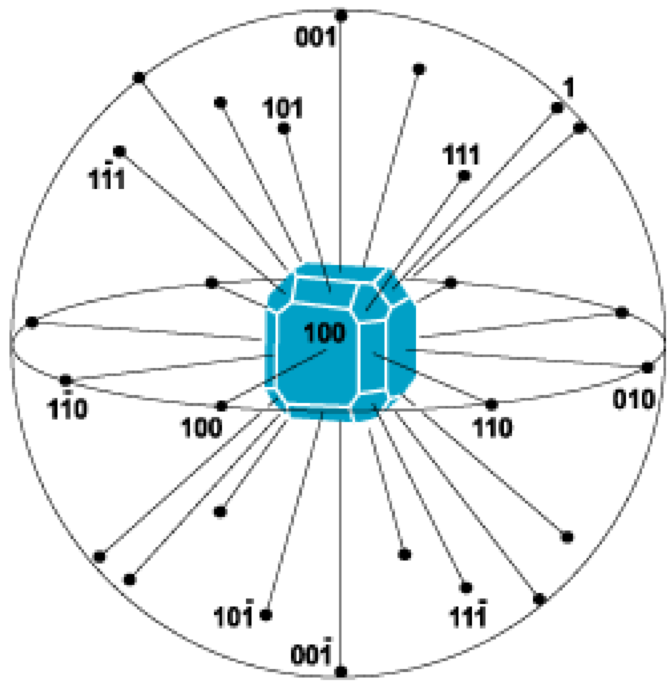


Fig. 4.3. Example of a reciprocal lattice, divided into layers along c^*.

Bragg's Law Rewritten

- $2d\sin(\theta)=n\lambda$
- $2\sin(\theta)/d^*=\lambda$
- $\sin(\theta)=d^*\lambda/2$
- $\sin(\theta)=(d^*/2)/(1/\lambda)$
- $|\mathbf{d^*}|=[h^2\mathbf{a^*}^2+k^2\mathbf{b^*}^2+l^2\mathbf{c^*}^2+2hk\mathbf{a^*b^*}\cos(\gamma^*)+2hl\mathbf{a^*c^*}\cos(\beta^*)+2kl\mathbf{b^*c^*}\cos(\alpha^*)]^{1/2}$
- If the reciprocal cell is known and the wavelength of the x-rays is known then the diffraction angle θ can readily be calculated for any set of hkl

Bragg Faces

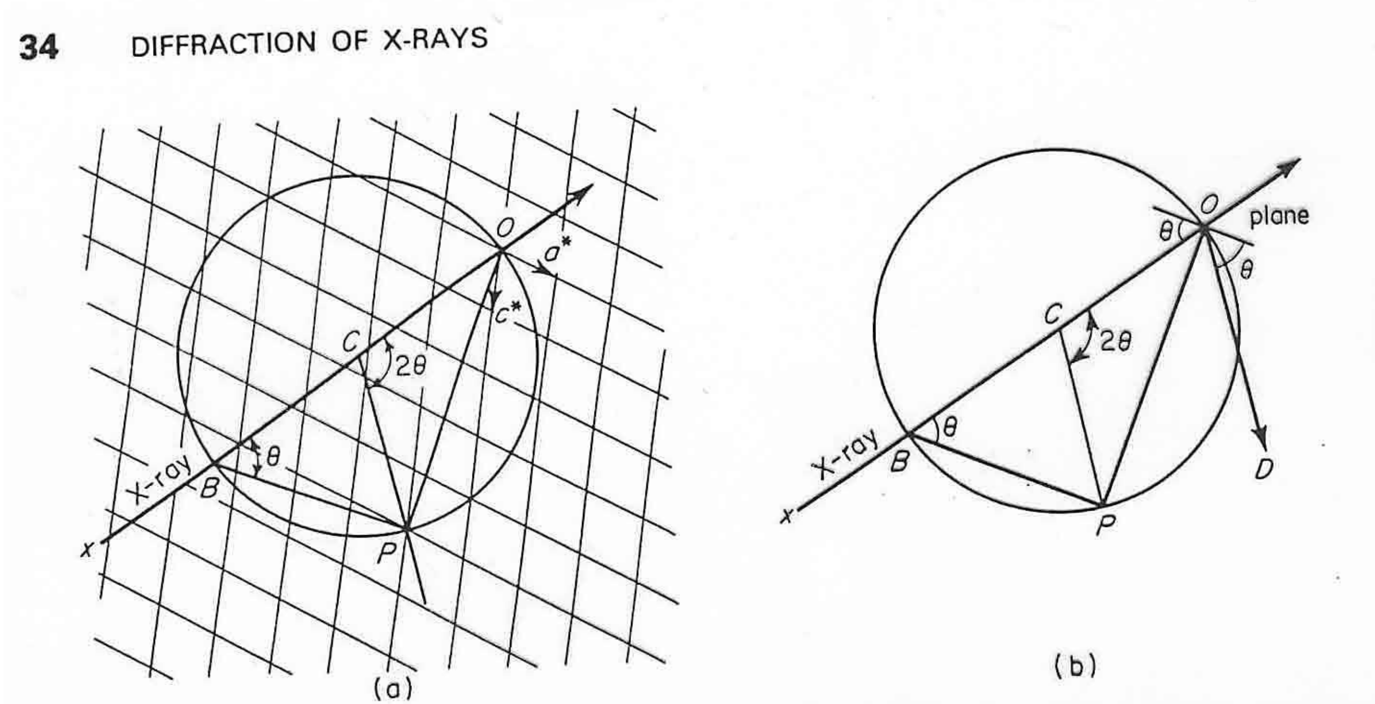


It makes no sense to talk of the 2,0,0 face but the 2,0,0 plane does make sense.

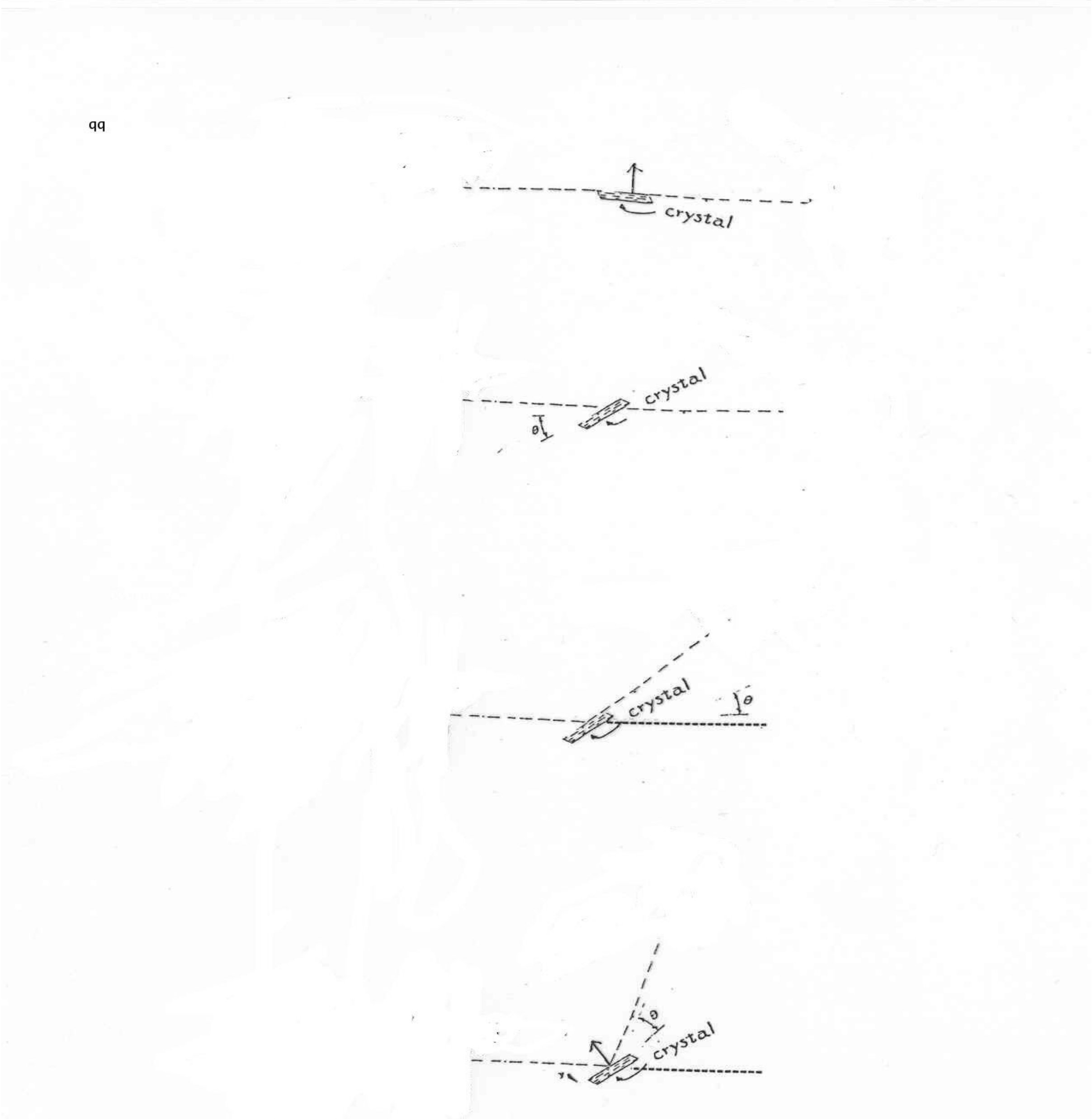
Uses of hkl

- Miller Indices
- A set of lattice planes
- A particular plane
- A crystal Face
- A direction in reciprocal space

The Ewald Sphere



Theta vs 2Theta



Homework 5

Using the monoclinic cell

a=15.168 b=10.348 c=15.847 alpha=90.0 beta=100.035 and gamma=90.0

- calculate:
  - The reciprocal cell constants—lengths and angles
  - The angle between **a** and **a***
  - The angle theta for the (2,5,2) reflection for copper radiation λ=1.54178.