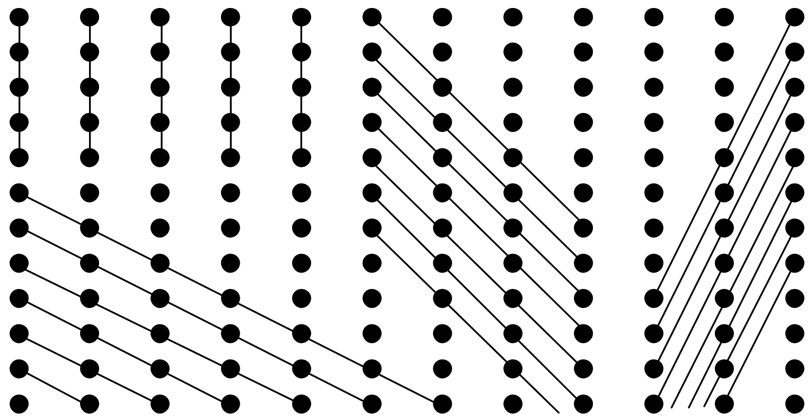
SOLID STATE 3

Crystal Planes and Diffraction

3.1 Crystal Planes

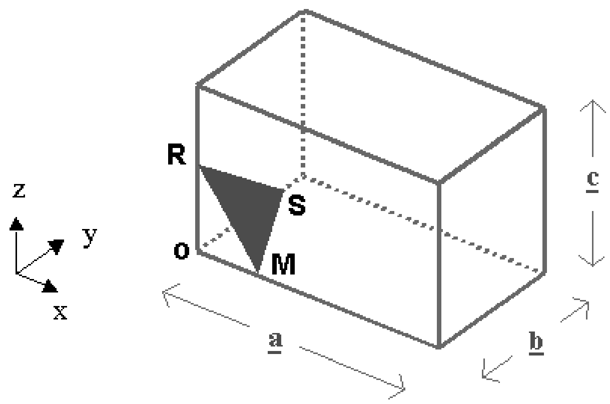
These are sets of parallel planes within a crystal. The distance between adjacent *lattice planes* is the *d-spacing*.



3.2 The Miller Index

The orientation of the planes is defined by the *Miller index* hkl

Example 1:

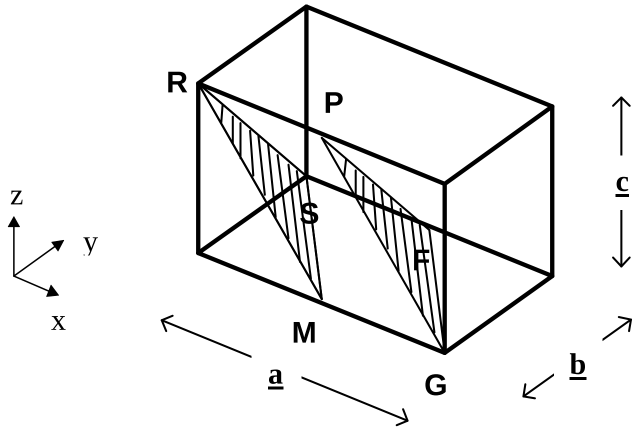


For plane RMS, the intercepts on *a*, *b* and *c* are	1/4, 2/3, 1/2
Take reciprocals to give	4, 3/2, 2
Round into integers if necessary	8 3 4
Miller Index for plane RMS	(8 3 4)

In reverse, a plane with Miller Index (h k l) has intercepts at $\frac{a}{h}\frac{b}{k}\frac{c}{l}$

Now, in the picture above the plane doesn't cut at a/8, b/3, c/4 - but one parallel to it does.

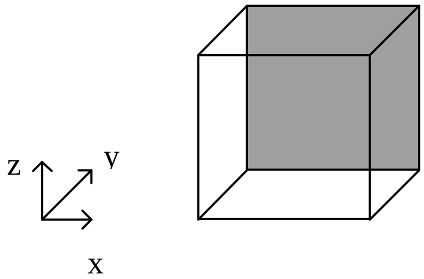
Example 2:



For plane RMS, the intercepts on *a*, *b* and *c* are ½, 1, 1
Take reciprocals to give 2 1 1
Round into integers if necessary 2 1 1
Miller Index for plane RMS (2 1 1)

3.3 Planes parallel to faces

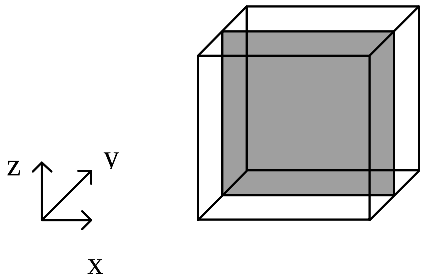
By the same method as described above, we can derive Miller indices for unit cell faces:



Intercepts: ∞ 1 ∞

Reciprocal: (0 1 0)

Plane perpendicular to x is (1 0 0)
Plane perpendicular to y is (0 1 0)
Plane perpendicular to z is (0 0 1)



Intercepts: ∞ ½ ∞

Reciprocal: (0 2 0)

Q1 Draw planes with Miller indices (1 0 0), (1 2 0), (1 2 3), (2 4 6)

3.4 Calculating the distance between planes

In orthogonal crystals, we can calculate the distance between planes, d, from the Miller index (h k l) and the unit cell dimensions *a,b,c* from the following formula

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

for ORTHOGONAL axes

Note that this can be simplified if *a*=*b* (tetragonal symmetry) or *a*=*b*=*c* (cubic symmetry).

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2}$$ for cubic,

$$\frac{1}{d^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$$ for tetragonal

Example: A cubic crystal has *a* = 5.2Å. Calculate the d-spacing of the (1 1 0) plane.

Note that the (1 1 0), (1 0 1), (0 1 1) (etc) planes all have the same d-spacing in this case.

Example: A tetragonal crystal has *a* = 4.7 Å, *c* = 3.4 Å. Calculate the separation of the:
(1 0 0), (0 0 1) and (1 1 1) planes.

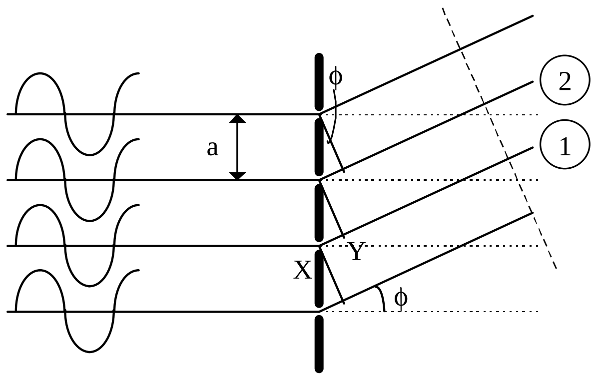
Note now that since $\mathbf{a} \neq \mathbf{c}$*, (100) is not the same as (001).*

Q2 If *a* = *b* = *c* = 8 Å, find d-spacings for planes with Miller indices (1 2 3)
Calculate the d-spacings for the same planes in a crystal with unit cell *a* = *b* = 7 Å, *c* = 9 Å.
Calculate the d-spacings for the same planes in a crystal with unit cell *a* = 7 Å, *b* = 8 Å, *c* = 9 Å.

(1 Å = 1 x 10^{-10}m)

3.5 Optical Diffraction Grating

A 1-dimensional analogue of X-ray diffraction
Coherent incident light impinges upon an evenly spaced grating; the parallel lines in the grating act as secondary light sources.



Coherent incident light Diffracted light

Path difference XY between diffracted beams 1 and 2:

$$\sin\phi = \frac{XY}{a} \quad \Rightarrow \quad XY = a \sin\phi$$

For 1 and 2 to be in phase and thus give constructive interference,

$$XY = \lambda, 2\lambda, 3\lambda, 4\lambda......n\lambda$$

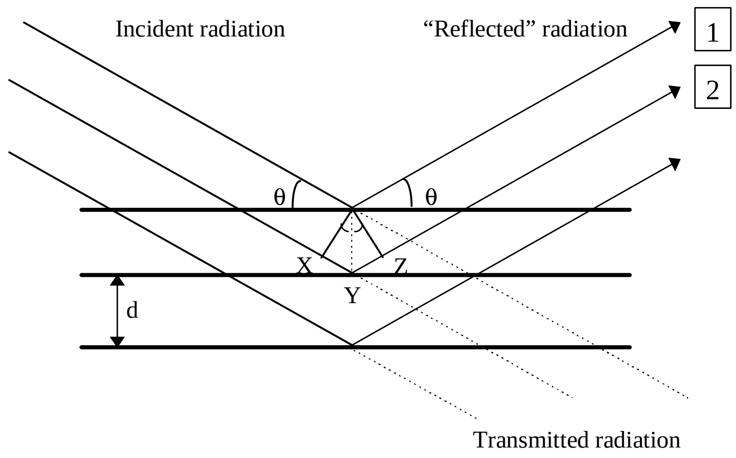
so

$$\boxed{a \sin\phi = n\lambda}$$

where n is the order of diffraction and must be an integer.

3.6 Bragg's Law

The planes in the crystal are considered to be reflecting planes



$$\mathbf{2d \sin \theta = n\lambda}$$

Bragg's law - where d = separation of planes, θ=angle of diffraction, λ=wavelength of X-rays and n is an integer.

We can rewrite this as:

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

if we adjust the Miller indices - see examples in lecture notes.

Example: X-rays with wavelength 1.54 Å are reflected from planes with d=1.2 Å. Calculate the Bragg angle θ for constructive intereference.

We can combine Bragg's Law and the d-spacing equation to solve a number of problems:

Example: X-rays with wavelength 1.54 Å are "reflected" from the (1 1 0) planes of a cubic crystal with unit cell a = 6 Å. Calculate the Bragg angle, θ, for all orders of reflection, n

CONCEPT QUESTIONS

3.1 Write down the d-spacing formula for orthogonal crystals.
3.2 How does this simplify for tetragonal and cubic symmetry?
3.3 What is the minimum value of a (in an optical grating) for first order diffraction to be observed?
3.4 What happens when $a << \lambda$? What happens when $a >> \lambda$?
3.5 What are the wavelength requirements for diffraction by a crystal lattice?
3.6 State Bragg's Law and explain the terms.
3.7 Explain why, in practice, n is set to 1 in the Bragg equation.

PROBLEMS

3.1 X-rays of wavelength λ=1.5Å are reflected from the (2 2 2) planes of a cubic crystal with unit cell a = 5Å. Calculate the Bragg angle, θ, for n=1.
3.2 The cubic crystal in the previous question is replaced with a tetragonal crystal, unit cell a = 4.5Å, c = 6Å. Calculate the Bragg angle, θ for the 222 reflection.
3.3 An orthorhombic crystal is now studied. What is the Bragg angle for the 222 reflection if a = 3Å, b= 3.5Å and c = 8Å