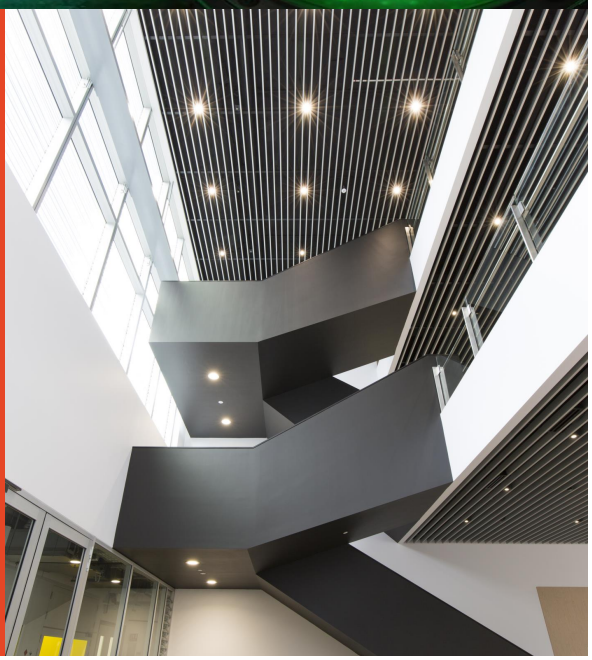
CMP Lecture 6

School of Physics
The University of Sydney



The reciprocal lattice

Solid State Basics Ch. 13

This is now formal but it is central to the whole of solid state physics.

The physics of waves in solids (vibrational and electron) is best described in reciprocal space (also called "k-space").
Can think of the reciprocal lattice as being a Fourier transform of the direct lattice.

Consider a set of points $\mathbf{R}$ constituting a Bravais lattice and a plane wave:

$$e^{i\boldsymbol{k}.\boldsymbol{r}}$$

For a general wave vector $\boldsymbol{k}$ such a wave will not have the periodicity of the Bravais lattice, but for certain special choices of wave vector it will.

The set of all wave vectors $\boldsymbol{G}$ that yield plane waves with the periodicity of a given Bravais lattice is known as its **reciprocal lattice.**

The reciprocal lattice

Analytically, $\boldsymbol{G}$ belongs to the so-called reciprocal lattice of a Bravais lattice of points

$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

provided $e^{i\boldsymbol{G}.(\boldsymbol{r}+\mathbf{R})} = e^{i\boldsymbol{G}.\boldsymbol{r}}$ for any $\boldsymbol{r}$ and all $\mathbf{R}$ in the Bravais lattice

That is, the **reciprocal lattice** is defined as the set of vectors $\boldsymbol{G}$ for which

$$e^{\mathbf{iG}\cdot\mathbf{R}} = 1 \quad \text{or} \quad \mathbf{R}\cdot\mathbf{G} = 2\pi l$$

(l is an integer) for all points $\mathbf{R}$ of the direct lattice

The reciprocal lattice is also a Bravais lattice

$$\mathbf{G} = m'\mathbf{b_1} + n'\mathbf{b_2} + o'\mathbf{b_3}$$

m', n', o' are integers

$\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ called **primitive reciprocal lattice vectors**

Note: instead of $\boldsymbol{G}$, sometimes $\boldsymbol{K}$ is used.

The reciprocal lattice

Note: the Bravais lattice that determines the given reciprocal lattice is often referred to as the "**direct lattice**"

Construction of the reciprocal lattice:

$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

$$\mathbf{G} = m'\mathbf{b_1} + n'\mathbf{b_2} + o'\mathbf{b_3}$$

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \qquad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \qquad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

cross-product

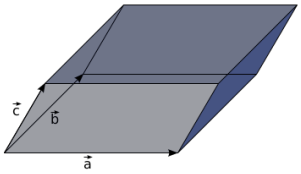
where

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

Kronecker $\delta_{ij} = 1$ for i=j, 0 otherwise

with this can see that

$$\mathbf{R}\cdot\mathbf{G} = 2\pi l$$



$\mathrm{V} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$

Volume of unit cell in real space

$\boldsymbol{R}.\boldsymbol{G} = (m\boldsymbol{a}_1 + n\boldsymbol{a}_2 + o\boldsymbol{a}_3).(m'\boldsymbol{b}_1 + n'\boldsymbol{b}_2 + o'\boldsymbol{b}_3)$

The reciprocal of the reciprocal lattice

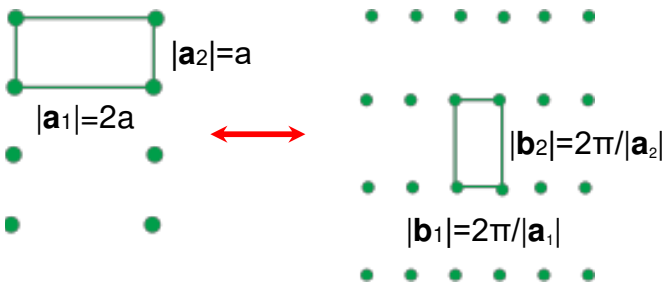
Since the reciprocal lattice is itself a Bravais lattice, we can construct its reciprocal lattice.

Its reciprocal lattice is just the original direct lattice!

If V is the volume of the primitive cell in direct (or real) space, then the primitive cell of the reciprocal lattice has a volume $(2\pi)^3/V$.

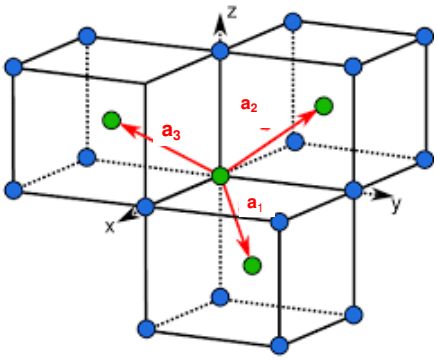
Worked example – 2D lattice

Consider a rectangular lattice in 2D with primitive lattice vectors (2a,0) and (0,a). Calculate the reciprocal lattice vectors for this lattice.



Find the reciprocal lattice of the simple cubic lattice

Find the reciprocal lattice of the bcc lattice

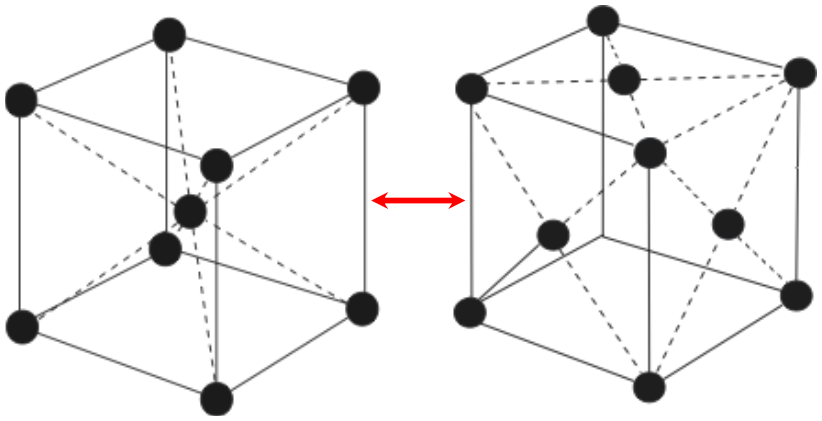


$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\boldsymbol{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$\boldsymbol{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

The reciprocal lattice



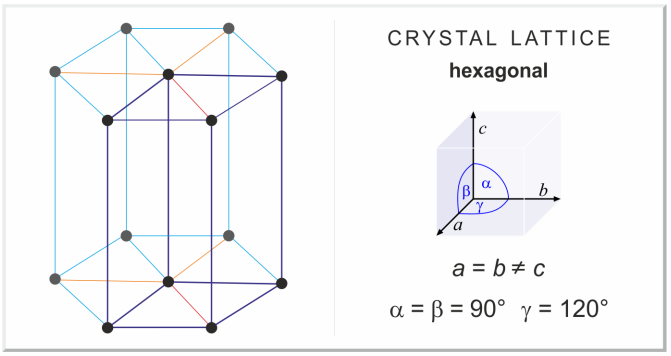
$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1(\mathbf{a}_2 \times \mathbf{a}_3)} \qquad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1(\mathbf{a}_2 \times \mathbf{a}_3)} \qquad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1(\mathbf{a}_2 \times \mathbf{a}_3)}$$

The **fcc lattice** is the reciprocal of the **bcc lattice** and vice versa.

Reciprocal lattice to the simple hexagonal Bravais lattice

The reciprocal to a simple hexagonal Bravais lattice with lattice constants *a* and *c* is another simple hexagonal lattice with lattice constants $4\pi/(\sqrt{3}a)$ and $2\pi/c$ rotated through 30° about the c-axis with respect to the direct lattice.

You will derive this in Quiz 3.

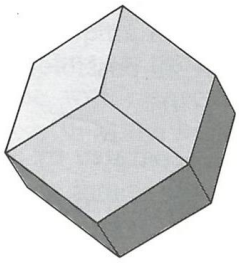


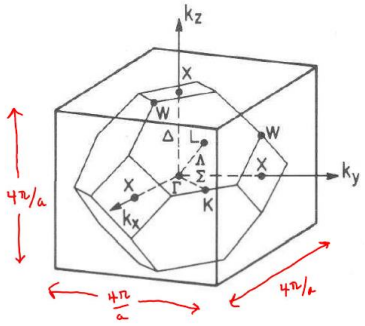
The first Brillouin zone

The Wigner-Seitz primitive cell of the reciprocal lattice is known as the **first Brillouin zone** (often just called the Brillouin zone, BZ).

Because the reciprocal of the bcc lattice is fcc, the first BZ of the bcc lattice is just the fcc Wigner-Seitz cell.

And since the reciprocal of the fcc lattice is bcc, the first BZ of the fcc lattice is the bcc Wigner-Seitz cell.

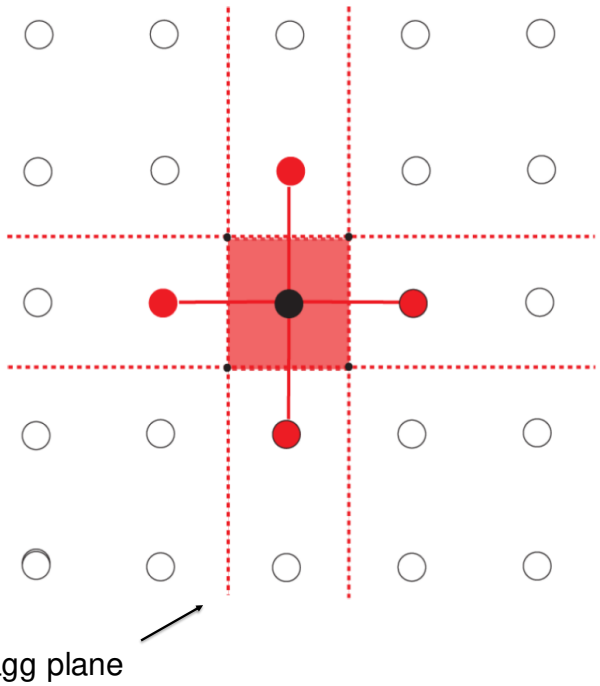




The letters and symbols represent high symmetry points and lines in the BZ

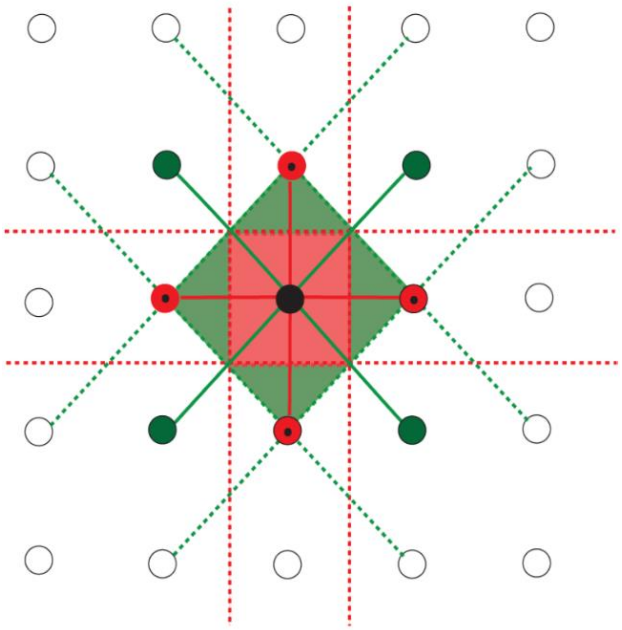
The first Brillouin zone

The locus of points in reciprocal space that have no Bragg planes between them and the origin defines the first Brillouin zone. It is equivalent to the Wigner-Seitz unit cell of the reciprocal lattice. Small black dots represent point of intersection of Bragg planes.



Higher Brillouin zones

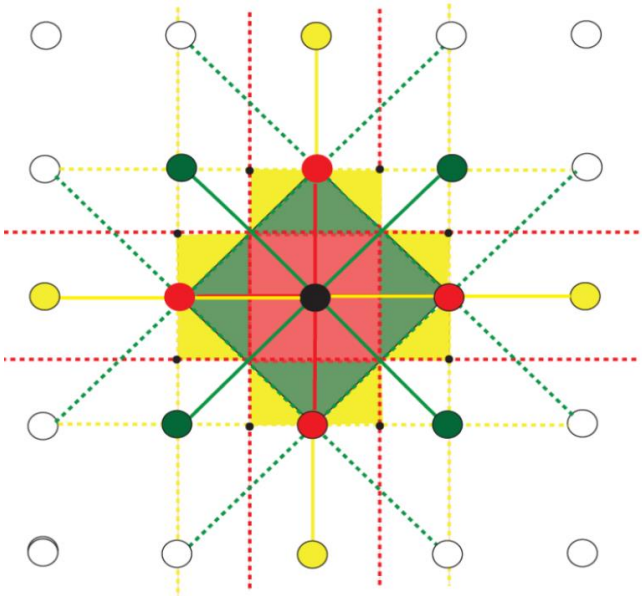
The second Brillouin zone is the region of reciprocal space in which a point has one Bragg plane between it and the origin. This area is shaded green in this picture. Note that the areas of the first and second Brillouin zones are the same. Small black dots represent points of intersection of Bragg planes.



Higher Brillouin zones

The construction can quite rapidly become complicated as you move beyond the first few zones, and it is important to be systematic so as to avoid missing out important Bragg planes.

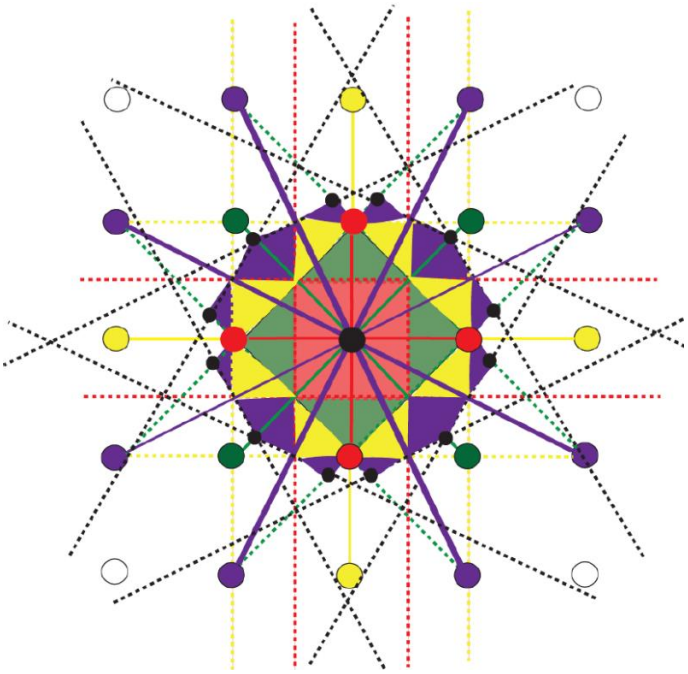
Yellow: 3rd BZ



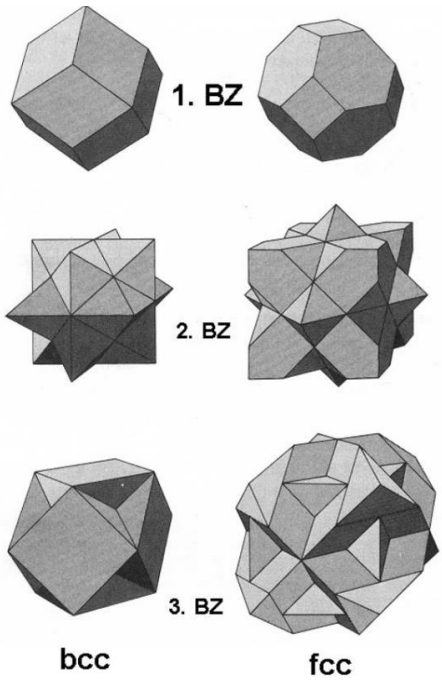
Higher Brillouin zones

Small black dots represent points of intersection of Bragg planes.

Purple: 4th BZ



First 3 Brillouin zones of bcc and fcc lattices



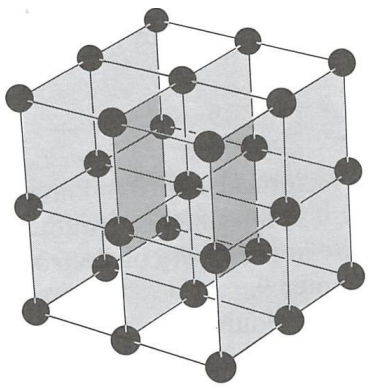
https://www.materialscloud.org/work/tools/seekpath

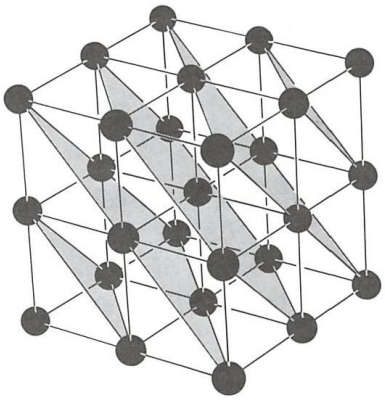
https://en.wikipedia.org/wiki/Bravais_lattice#In_3_dimensions

Lattice planes

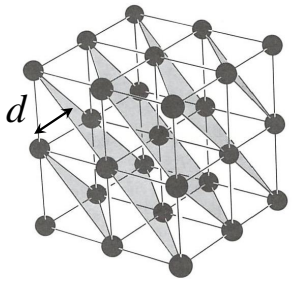
A **lattice plane** (or *crystal plane*) is a plane containing at least three noncolinear, and therefore infinite number of points of a lattice.

A **family of lattice planes** is an infinite set of equally separated lattice planes which taken together contain all points in the lattice.





Lattice planes



For any family of lattice planes separated by a distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which has a length of $\mathbf{G}=2\pi/d$.

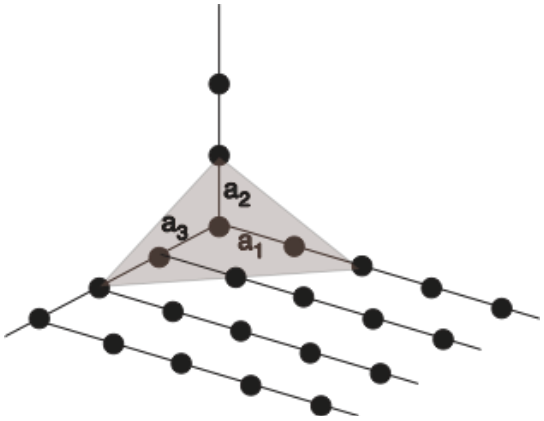
Conversely, for any reciprocal lattice vector **G**, there is a family of lattice planes normal to **G** and separated by a distance d, where $2\pi/d$ is the length of the shortest reciprocal lattice vector parallel to **G**.

Miller indices of lattice planes

- We use the shortest such reciprocal lattice vector to arrive at the **Miller indices** of the plane (common notation).
- Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vectors normal to that plane, with respect to the specified set of primitive reciprocal lattice vectors.
- A plane with Miller indices *h, j, l* is normal to the reciprocal lattice vector $\mathbf{G} = h\,\mathbf{b}_1 + k\,\mathbf{b}_2 + l\,\mathbf{b}_3$.
- *h, k, l* are integers.
- They have no common factor.
- They depend on particular choice of primitive vectors.

Labelling crystal planes (Miller indices)

Describes the orientation of a plane by giving a vector normal to the plane.



1. Determine the intercepts with the axes in units of the lattice vectors.
2. Take the reciprocal of each number.
3. Reduce the numbers to the smallest set of integers having the same ratio. These are then the **Miller indices**.

step 1: (2,1,2)

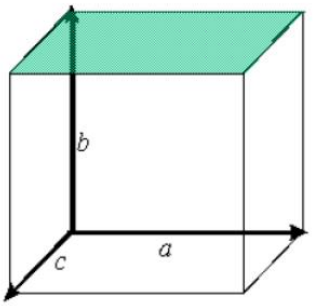
step 2: (1/2,1,1/2)

step 3: (1,2,1)

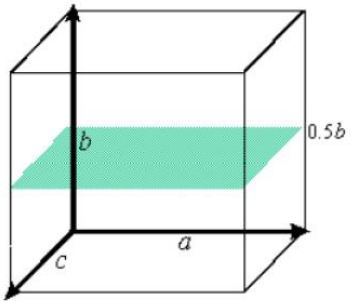
Miller indices is a set of integers with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes.

Examples of Miller indices

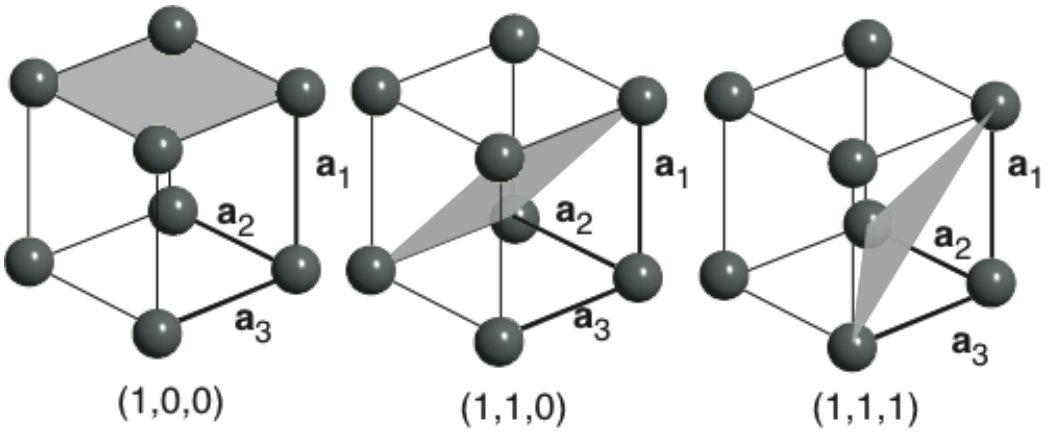
1.



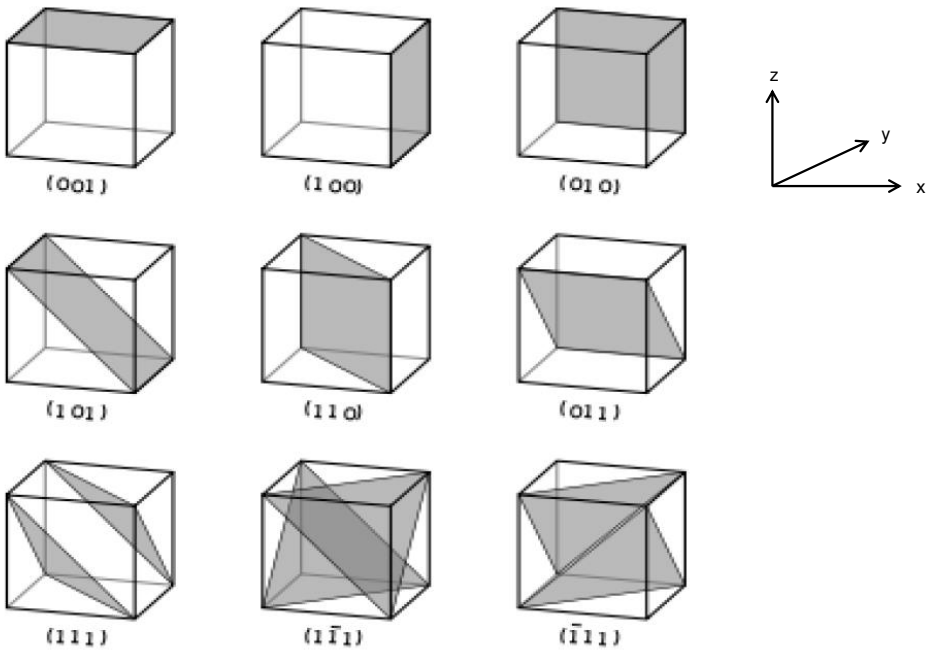
2.



Examples



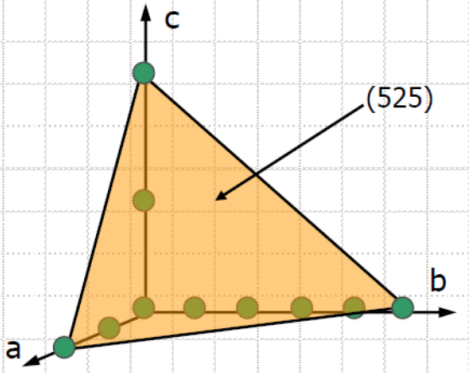
More examples



$\bar{1} = -1$ Usual to use "bar" instead of negative sign

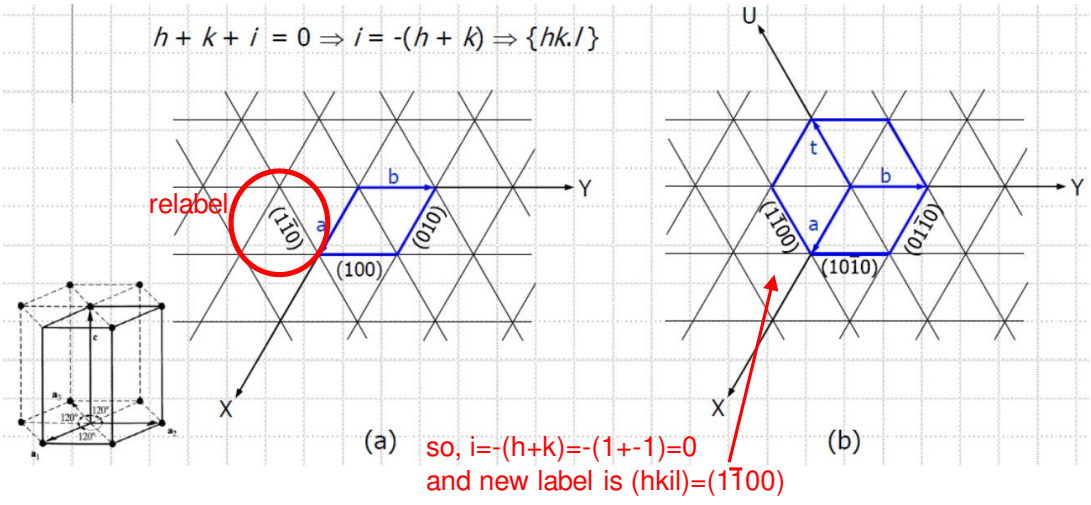
Another example

	a	b	c
The intercepts	2	5	2
The reciprocals	1/2	1/5	1/2
Multiply by 10	5	2	5
The Miller indices	(525)		



Special case: trigonal & hexagonal lattice

- (11$\bar{0}$), (100), and (010) are indices different in type but describe crystallographically equivalent lattice planes.
- Introducing the fourth axis U. We have Miller-Bravais indices (*hkil*).
- All indices of the planes are of the same form {10$\bar{1}$0}.



Lattice plane spacings

Spacing between adjacent planes of a family of planes specified by Miller indices *(h,k,l)*:

$$\mathbf{G}_{(h,k,l)} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$$

Then:

$$d_{(hkl)} = \frac{2\pi}{|\mathbf{G}|} = \frac{2\pi}{\sqrt{h^2|\mathbf{b_1}|^2 + k^2|\mathbf{b_2}|^2 + l^2|\mathbf{b_3}|^2}}$$

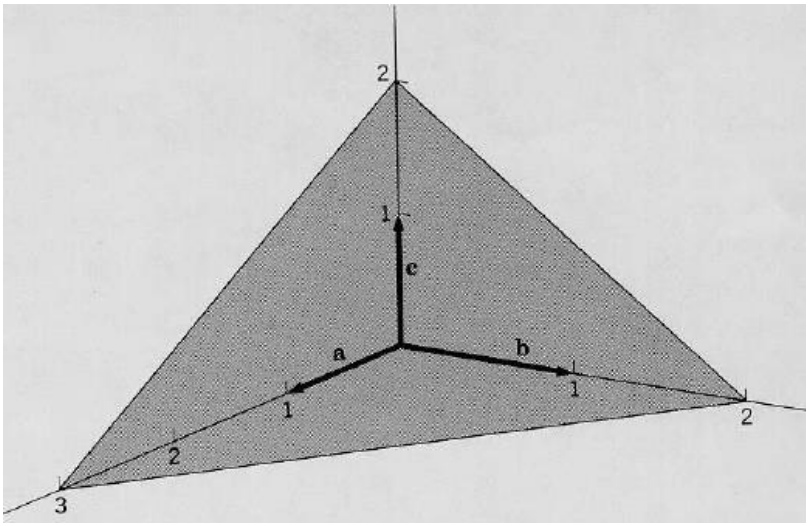
assuming that the lattice vectors $\mathbf{b}_i$ are orthogonal.
Since $|\mathbf{b}_i|=2\pi/|\mathbf{a}_i|$, then:

$$\frac{1}{|d_{(hkl)}|^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}$$

and for a cubic lattice:

$$d_{(hkl)}^{cubic} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

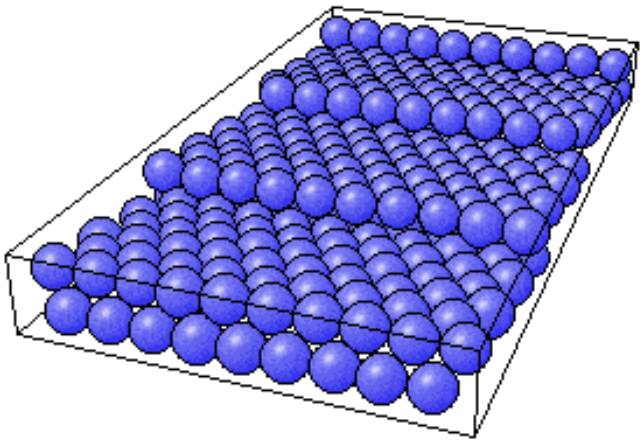
Example



Notation: family of planes

- (100), (010) and (001) planes are equivalent in a cubic crystal; including $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$.
- We refer to them collectively as the {100} planes, and in general we use {*hkl*} to refer to the (*hkl*) planes and all those that are equivalent to them by virtue of the crystal symmetry.

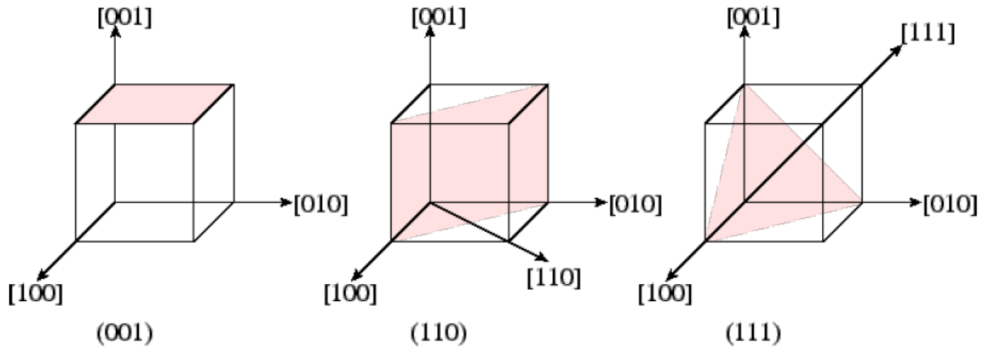
Example of a high Miller-index surface



fcc(775) surface

Notation: directions and family of directions

A similar convention is used to specify directions in the direct lattice, but to avoid confusion with the Miller indices (directions in the reciprocal lattice) square brackets are used instead of parenthesis.



The [100], [010], [001], [100], [010] and [001] directions in the cubic crystal are referred to, collectively, as the <100> directions.

Exercise: list the directions belonging to <111> (should find 8)

Visualizing crystal planes

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/crystalstructure.php

End