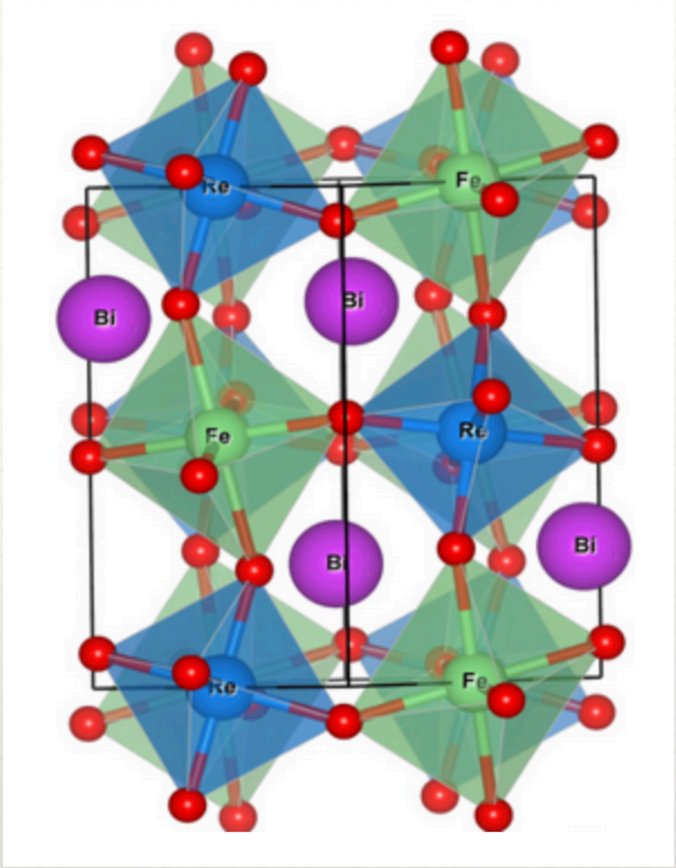


Structure of Solids - Axes, Planes, Directions

Lecture 2

CHM 637
Chemistry & Physics of Materials

Varadharajan Srinivasan
Dept. Of Chemistry
IISER Bhopal

Lecture Plan

- Brief introduction to Crystal Symmetry
- Lattice axes, planes and directions

Crystal Symmetry

Crystallographic Point Groups

Collection of (non-translational) internal symmetries - axes of rotations, mirror planes, inversion, etc.

Only 32 combinations of point symmetry elements found in crystals. Each combination is called a point group or a crystal class.

Only molecules or groups of atoms (unit cell) that belong to these point groups can be repeated periodically.

Point groups of crystals can be extremely important in determining their properties.

Crystal Symmetry

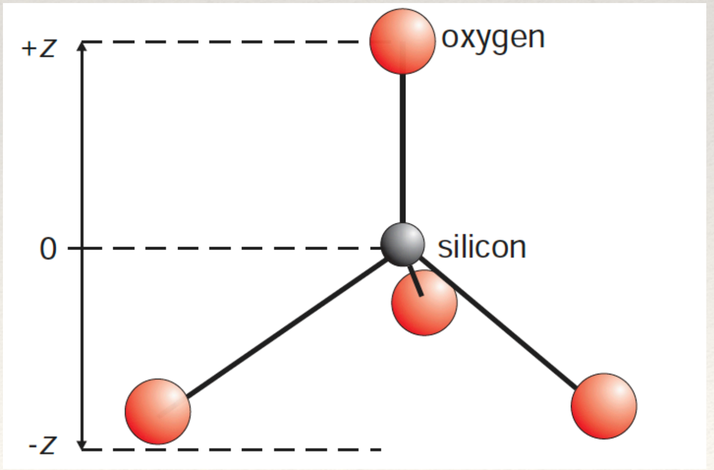
Crystallographic Point Groups

E.g. Piezoelectricity is only found in crystals that lack a centre of symmetry (non-centrosymmetric crystals)

Centre of inversion at (0,0,0) => If there is an atom at the point (x,y,z) then there is also an atom (of the same kind) at (-x, -y, -z).

Systems with no centre of symmetry have one or more polar axes which are unique.

Any atom on such an axis, say at z, does not have an equivalent at -z.



Crystal Symmetry

Space Groups

In additional to point symmetries there can be translational symmetry elements like glide planes and screw axes which yield equivalent structures but do not keep any point invariant.

Put together the translational and non-translational symmetries allow for 230 symmetry groups that can be repeated in space. These are the 230 Space Groups.

Notation for space groups: e.g. **P** m3m → List of essential (transl. and non-trans.) symmetry elements

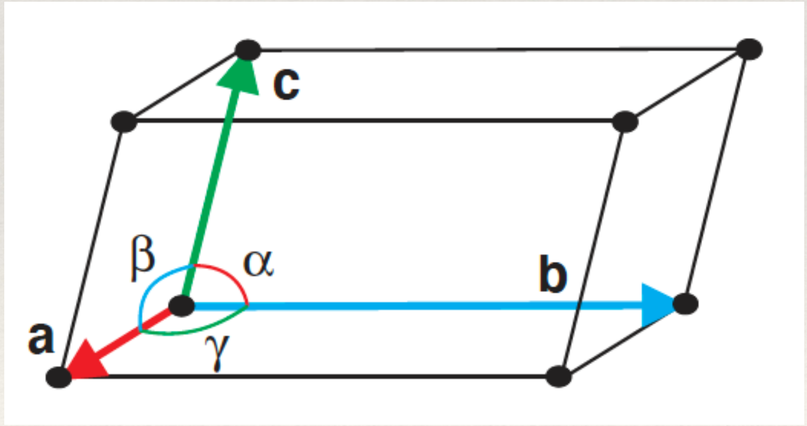
Unit cell type - **P**=primitive
I=body-centred
F=face-centred
C=base-centred

Lattice Axes, Planes and Directions

Lattice Axes

There is no unique choice of lattice axes (**a**, **b** and **c**).

Conventionally, the lattice axes are taken to lie along the unit cell edges.



Lattice Axes, Planes and Directions

Lattice Planes

Atomic planes in a crystal are very important especially in diffraction studies.

They are usually specified by Miller indices. These are decided as follows :

1. Three lattice points falling on the plane are located.

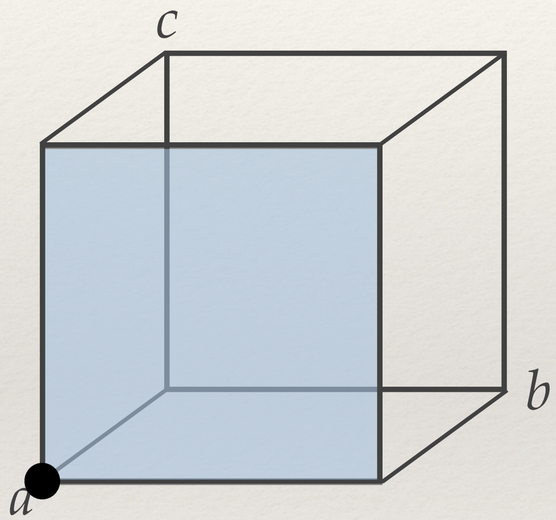
2. Their intercepts on the lattice axes are noted in units of the corresponding cell length.

3. Reciprocal of these numbers are taken.

4. Reciprocals are multiplied by the LCM to yield the Miller indices

Lattice Axes, Planes and Directions

Lattice Planes



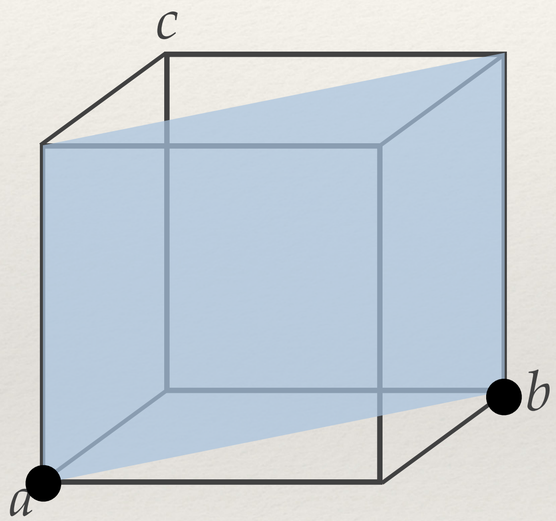
Intercept at (1,∞,∞)

Reciprocal (1,0,0)

Miller index (1,0,0)

Lattice Axes, Planes and Directions

Lattice Planes



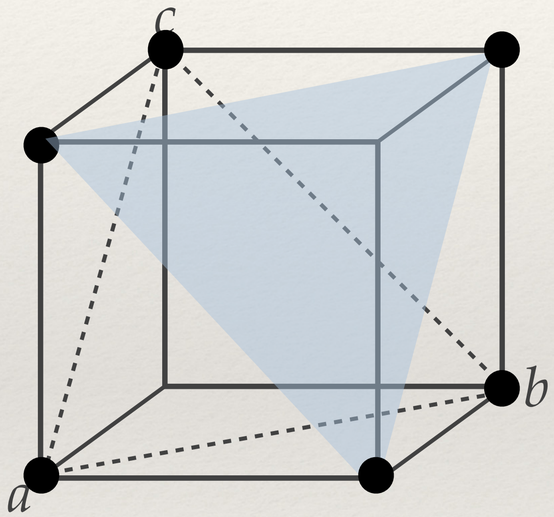
Intercept at (1,1,∞)

Reciprocal (1,1,0)

Miller index (1,1,0)

Lattice Axes, Planes and Directions

Lattice Planes



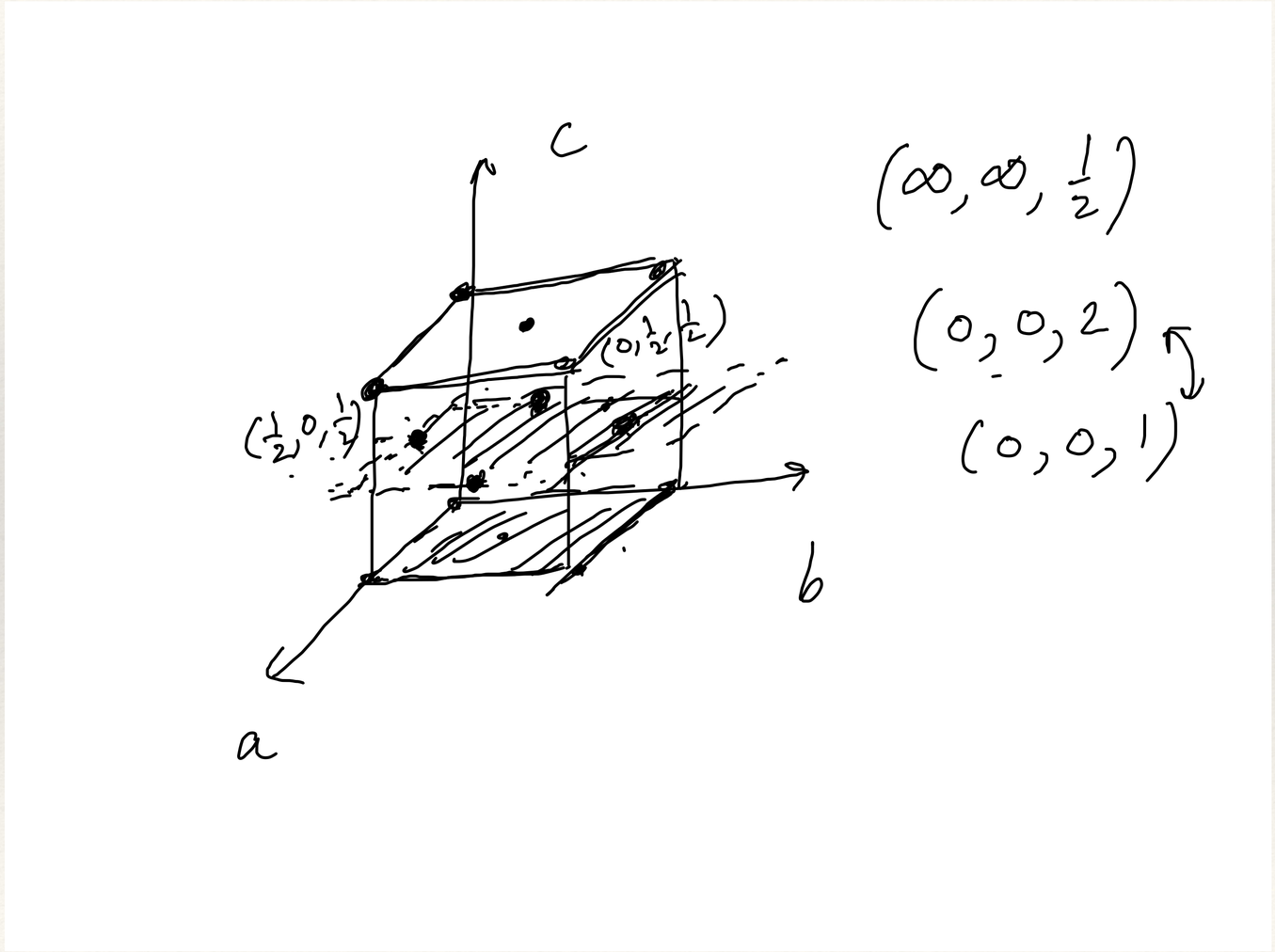
Intercept at (1,1,1)

Reciprocal (1,1,1)

Miller index (1,1,1)

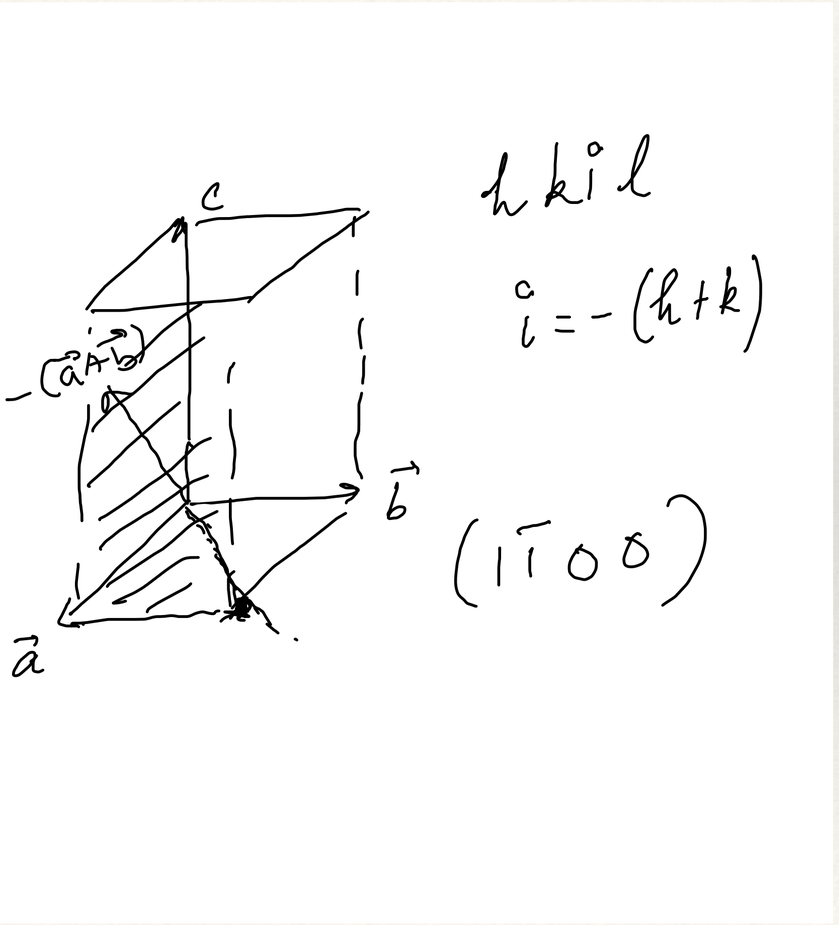
Lattice Axes, Planes and Directions

Lattice Planes



Lattice Axes, Planes and Directions

Lattice Planes



Lattice Axes, Planes and Directions

Lattice Planes

1. The Miller indices (*hkl*) correspond to a set of identical parallel lattice planes in the crystal.
2. For cubic lattices the perpendicular distance between adjacent parallel planes is given by

$$d = a/\sqrt{h^2 + k^2 + l^2}$$

3. When a lattice plane is parallel to one of the lattice axes, the corresponding intercept is taken to be at infinity and the corresponding Miller index is zero.
4. A lattice plane with a negative intercept has a negative Miller index denoted by a bar over it.

Lattice Axes, Planes and Directions

Lattice Planes

5. {*hkl*} refers to a family of symmetry related planes. E.g. {100} are 6 faces of cubic unit cell.
6. Important lattice planes are those will lower Miller indices, since these planes have the highest concentration of atoms.
7. For hexagonal lattices there are 4 axes to consider.

Lattice Axes, Planes and Directions

Lattice Directions

Direction from the origin to a lattice point at

$$\vec{R}_{lmn} = l\vec{a} + m\vec{b} + n\vec{c}$$

is referred to as the [*l m n*] direction.

Direction indices - The smallest set of integers *l m n* corresponding to a given direction

In cubic crystals the (*h k l*) planes are perpendicular to the [*h k l*] direction.

A set of lattice directions related by symmetry are referred to as <*l m n*>

Lattice Axes, Planes and Directions

Lattice Directions