Tutorial 1

1. (a) What is a semiconductor?

(b) Which are the 2 main properties that distinguish the semiconductor from a conductor?

(b) The bandgaps of semiconductors range typically between which values of energy and absorb in which wavelength range?

Energy:

Wavelength:

(c) What are the 2 types of bandgaps that we can find in semiconductors? Draw diagrams.

(d) In which groups of the Periodic Table of Elements can we find semiconductor materials?

(e) Most common crystal structures for semiconductors (the basic ones)?

2. Recall the concepts of Lattice and Bravais Lattice. What is the difference between them?

Answers

Lattice means 'order' and is a pure mathematical concept to describe ordered structures. It obeys well defined rules and properties. The concept can be used or applied to varied domains in science.

*Bravais Lattice merges the concept of Lattice (pure mathematical entity) and Base (physical entities positioned at the lattice points. Lattice concept applied to ordered Solid State structures: crystallography

A lattice to be *Bravais type* has to additionally obey certain criteria:
*be an infinite array of discrete points in three dimensional space generated by a set of discrete translation operations described by the following vector:

$\vec{R} = n\vec{u}_1 + m\vec{u}_2 + l\vec{u}_3$

n, m, l are integers and represent **lattice points**

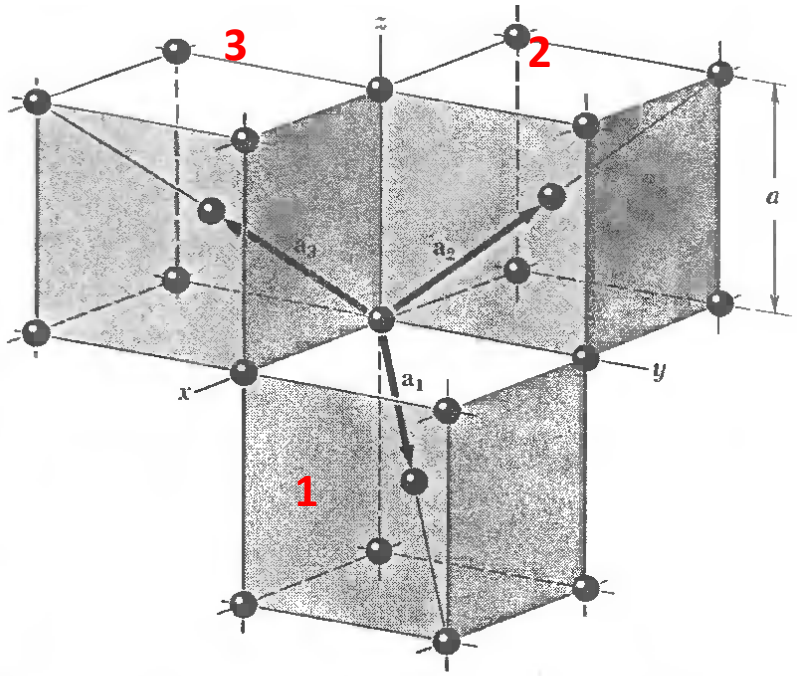
$\vec{u}_1$, $\vec{u}_2$, $\vec{u}_3$ are vectors, called **primitive vectors** along the 3 directions of space.

In 3D space a translation of the whole lattice by any *translation vector* given by this vector **leaves the lattice unchanged**.

3. In the following figure ID: lattice points and primitive vectors?
4. Write the primitive vectors for each lattice.
5. ID the Bravais Lattice. Is it a Unit cell or a Primitive Unit cell? Why?
6. What is *a* ?
7. Draw the Primitive Unit Cell. (see lecture 2 - **Homework**)

Answers

3. Lattice points: all black round dots
priminitive vectors: $\overrightarrow{a_1}$, $\overrightarrow{a_2}$, $\overrightarrow{a_3}$



4.

$$\overrightarrow{a_1} = \frac{1}{2}a\left(\overrightarrow{u_x} + \overrightarrow{u_y} - \overrightarrow{u_z}\right)$$

$$\overrightarrow{a_2} = \frac{1}{2}a\left(-\overrightarrow{u_x} + \overrightarrow{u_y} + \overrightarrow{u_z}\right)$$

$$\overrightarrow{a_3} = \frac{1}{2}a\left(\overrightarrow{u_x} - \overrightarrow{u_y} + \overrightarrow{u_z}\right)$$

5. Bravais Lattice: body centered cubic (bcc)
It's a Unit Cell with a 2 point basis to take advantage of the cubic symetry! A **Primitive Unit Cell** in solid state physics is a minimum volume cell corresponding to a single lattice point (1 point basis) of a structure with discrete translational symmetry.

6. a = lattice constante

8. Homework:
Do the same for the fcc.

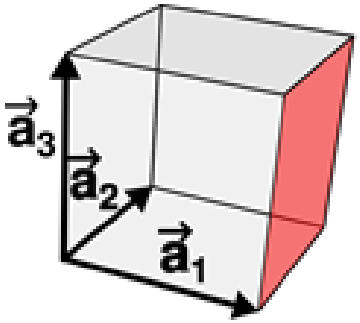
7. What are the Miller indices? How are they determined?

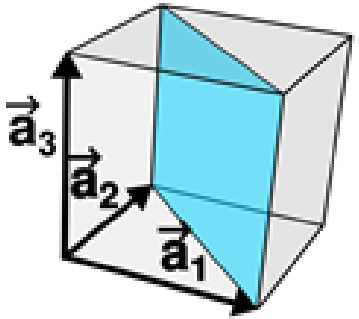
- The Miller indices is a notation system in crystallography for planes in crystal (Bravais) lattices.

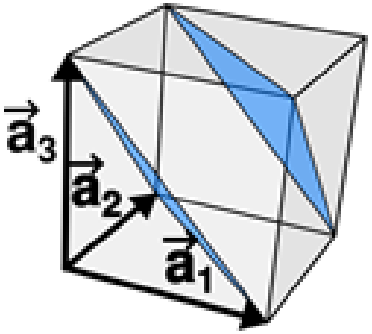
- It's a set of three integer numbers or letters: h, k, ℓ used to indicate the position of a face, an internal plane of a crystal or family of crystal planes, determined on the basis of the reciprocal of the intercept of the face or plane on the crystallographic axes is a set of Miller indices.

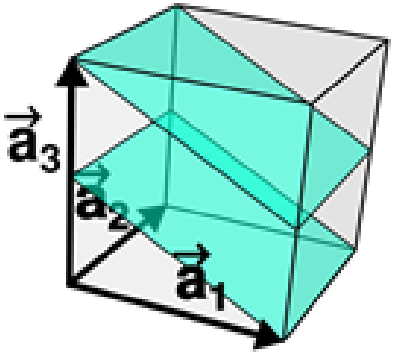
(1) choose a plane not pass through (0, 0, 0)
(2) determine the intercepts of the plane with x, y, and z axes
(3) form the reciprocals of these intercepts
(4) find the smallest set of whole numbers that are in the same ratio as the intercepts

8. Find the Miller indices for the following examples?









(100)

(110)

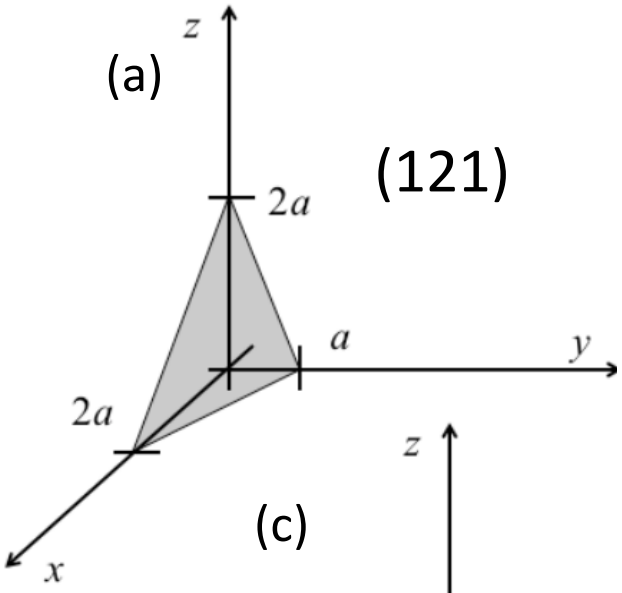
(111)

(102)

Axis intercept: 1, ∞, ∞
Reciprocal of intercept pts: 1, 0, 0
Miller indices: (100)

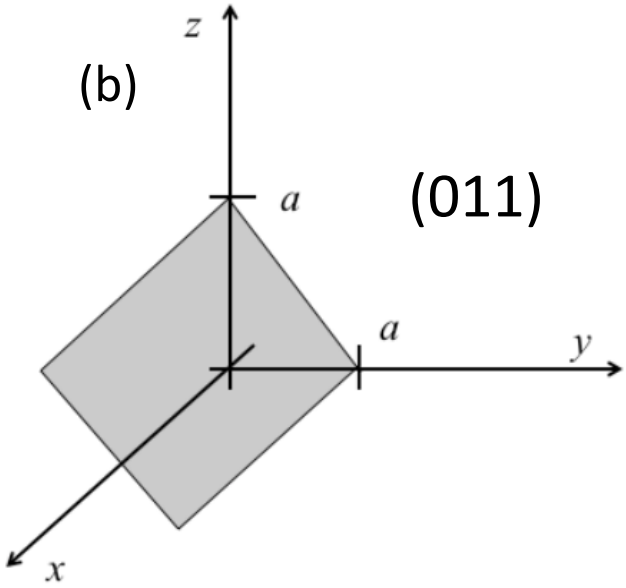
9. Find the Miller indices for the following examples?

(a)



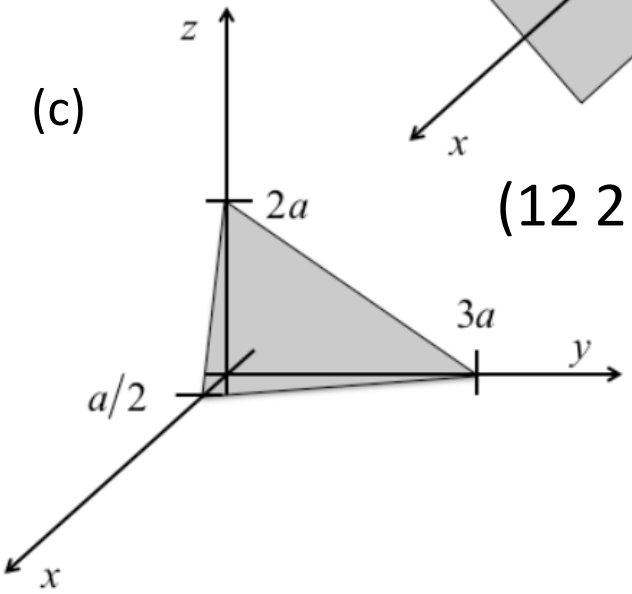
(121)

(b)



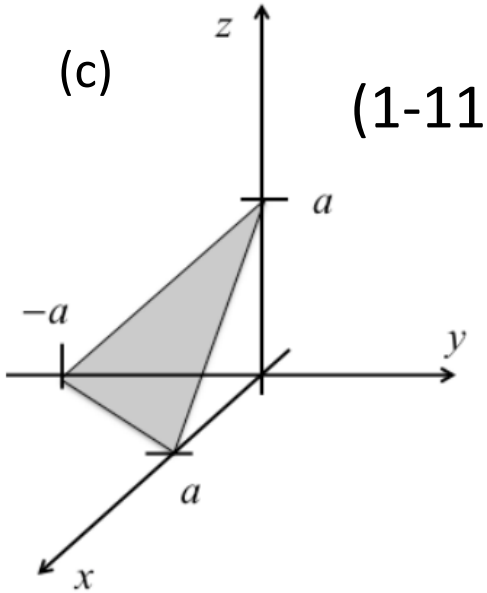
(011)

(c)



(12 2 3)

(c)



(1-11)

10. a) Assuming that the cristal constant for the previous situations is *a*, calculate the interplanar spacing between two closest parallel planes with the same Miller indices.

10. b) Draw examples or find 2 good examples of 2 planes in the above conditions.

a) The interplanar spacing between 2 closest planes belonging to the same familly is given by:

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

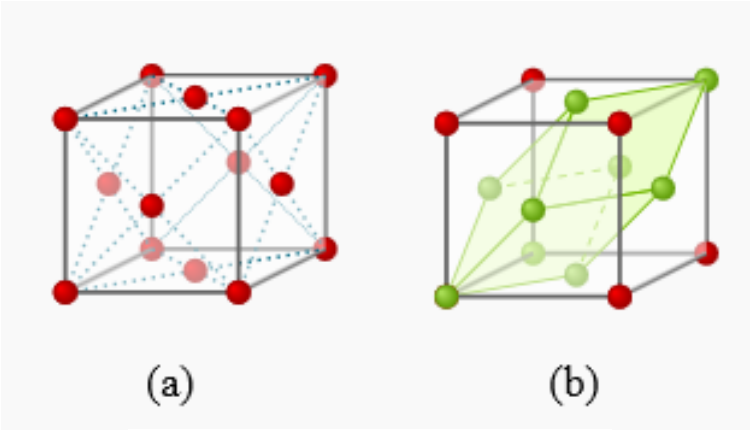
b) For 2 planes to belong to the same familly they must be parallel to each other and the distance between them must be given by the above expression, which depends on the Miller indices of the familly of planes to which they belong. For example the 2 planes planes in the 3rd and 4th cube in question 8. For the 3rd cube this distance is d = a/$\sqrt{3}$; for the 4th cube this distance is d = a/$\sqrt{5}$.

11. Consider the fcc cell.

a) What is the number of lattice points per unit cell?

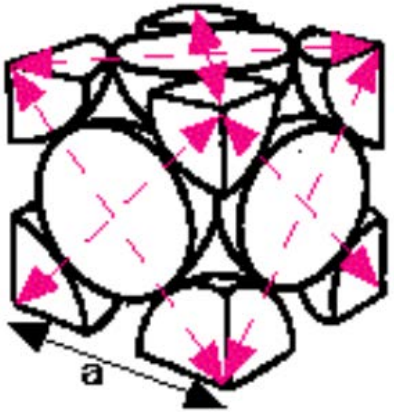
b) What is the coordinaton number?

c) What is the Atomic Packing Factor or packing density of the fcc cell?

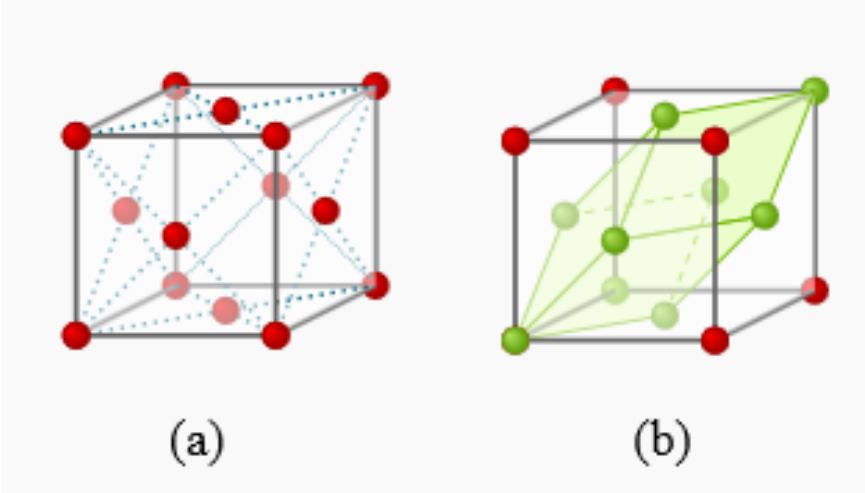


11 a) The 8 vertices are shared by 8 cells and contribute therefore only with 1/8 each (think of them as extended spheres). The 6 additional points at the faces are shared by two cells and therefore contribute with 1/2 respectively. So this adds up to a total of :

$$n = 8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2} = 4$$



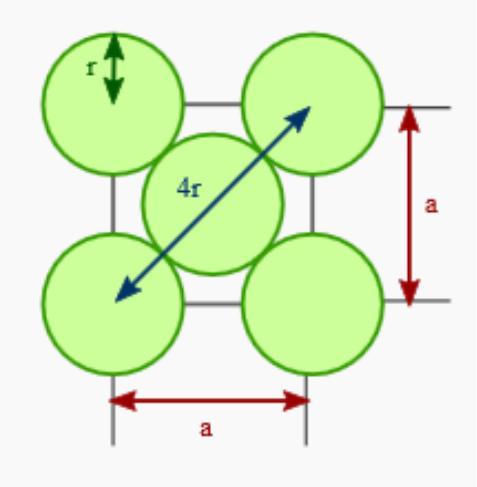
b) The coordination number, also called ligancy, of a central atom in a molecule or crystal is the number of atoms, molecules or ions bonded to it. In this case we can calculate it in 2 ways…….



b) The coordination number, also called ligancy of a central atom in a crystal is the number of atoms, molecules or ions bonded to it. In this case we can calculate it in 2 ways:

1-considering the nr. of atoms bonded to the atom located in the vertice.
For this case we see that in the fcc structure the face centered atoms are the nearest atoms so one corner atom is surrounded by 4 faces in X plane, 4 faces Y plane and 4 faces in Z plane: 4 x 3=12 face centered atoms, so co-ordination number is 12.

2- considering the nr. of atoms bonded to the atom located in the center of one face.
This atom is surrounded by 4 corner atoms of its own plane atoms, and the adjacent face centered atoms that is 8: 4+8 = 12 so the co-ordination no. is 12.



11 d) When the lattice points are inflated gradually, at some point they start to touch each other along the diagonals of the faces of the cube. One can now interpret them as close packed spheres with a radius defined geometrically by:

$$4r = \sqrt{2}a \Leftrightarrow \; r = \frac{\sqrt{2}}{4}a$$

The APF or the *packing density* ϱ is the ratio of the volume filled by the spherical atoms within a unit cell to the total volume Vuc of the unit cell:

$$\text{APF} = \frac{\dfrac{\text{atoms}}{\text{unit cell}} \cdot \dfrac{\text{volume}}{\text{atom}}}{\dfrac{a^3}{\text{volume}\,/\,\text{unit cell}}} = \frac{4 \cdot \frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3}{a^3}$$

Homework:

Do the same for the bcc.