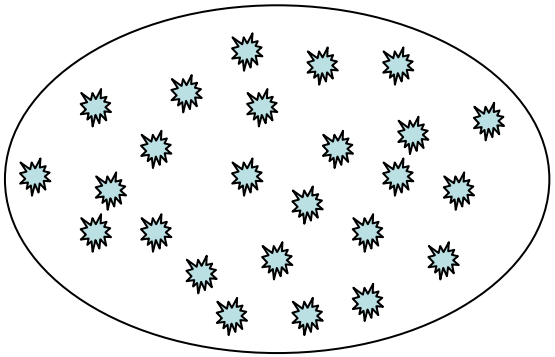
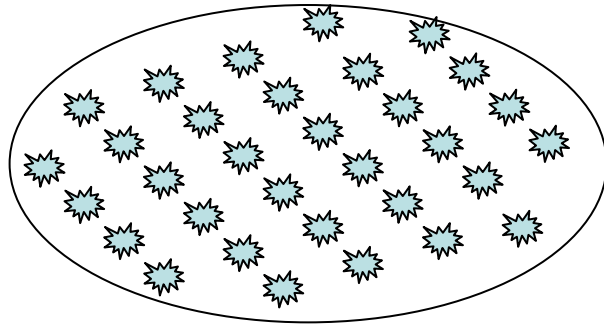
Classification of Solid Structures

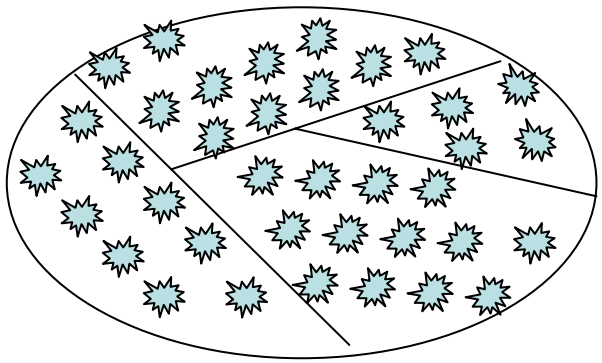


Represents an atom or a molecule



Amorphous: Atoms (molecules) bond to form a very short-range (few atoms) periodic structure.

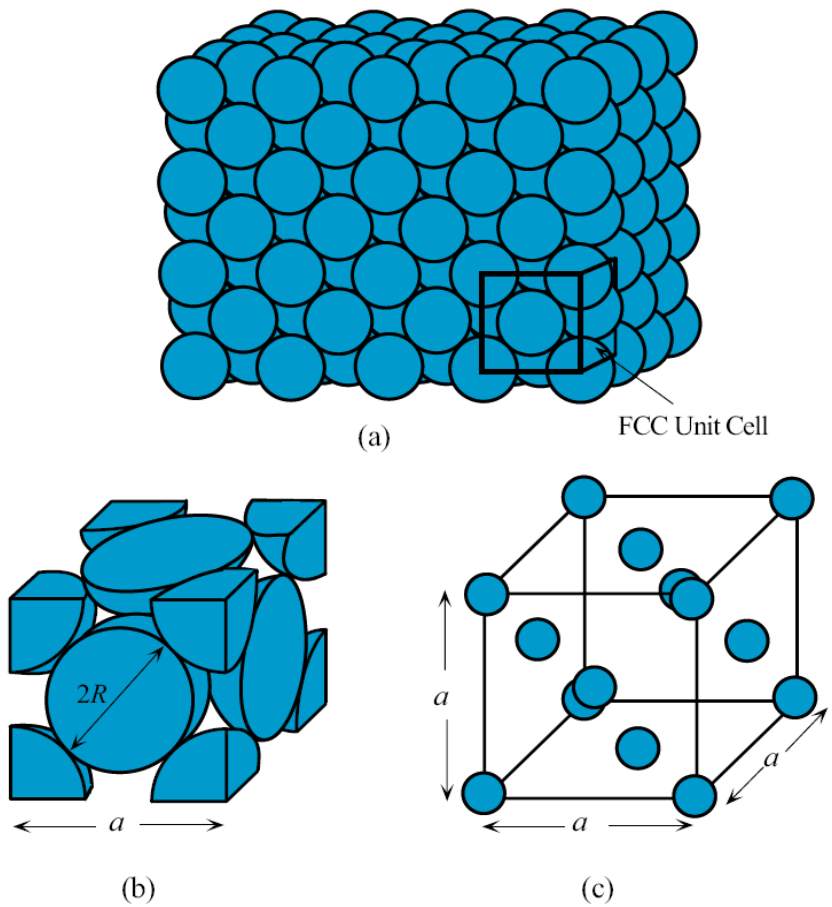
Crystals: Atoms (molecules) bond to form a long-range periodic structure. The constant bonds (coordination) , bond distance and angles between bonds are the characteristics of a crystal structure



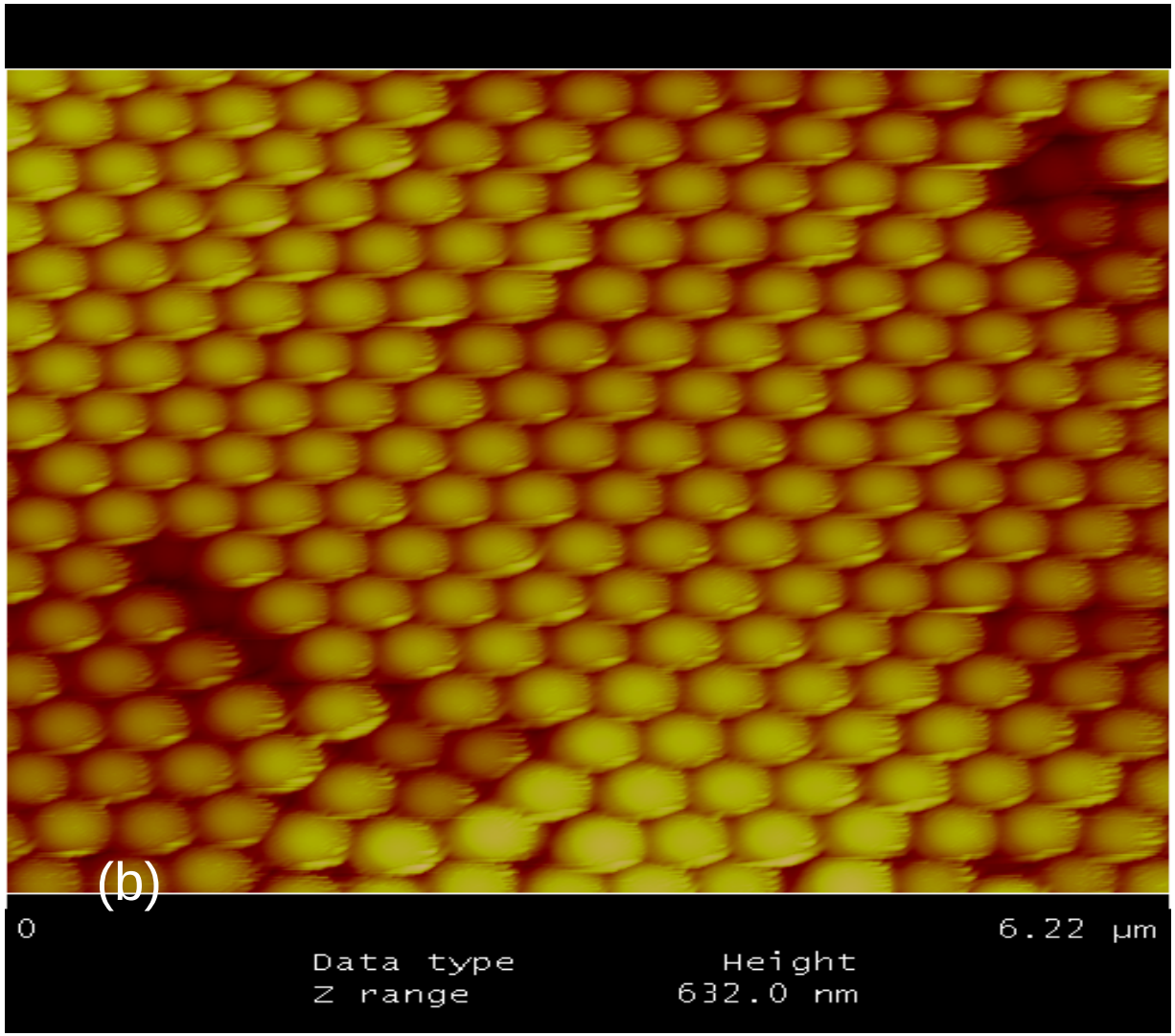
Polycrystalline: made of pieces of crystalline structures (called grain) each oriented at different direction (intermediate-range-ordered)

Crystals

An IDEAL CRYSTAL is constructed by the infinite repetition of identical structural units in space.



Crystalline Structures



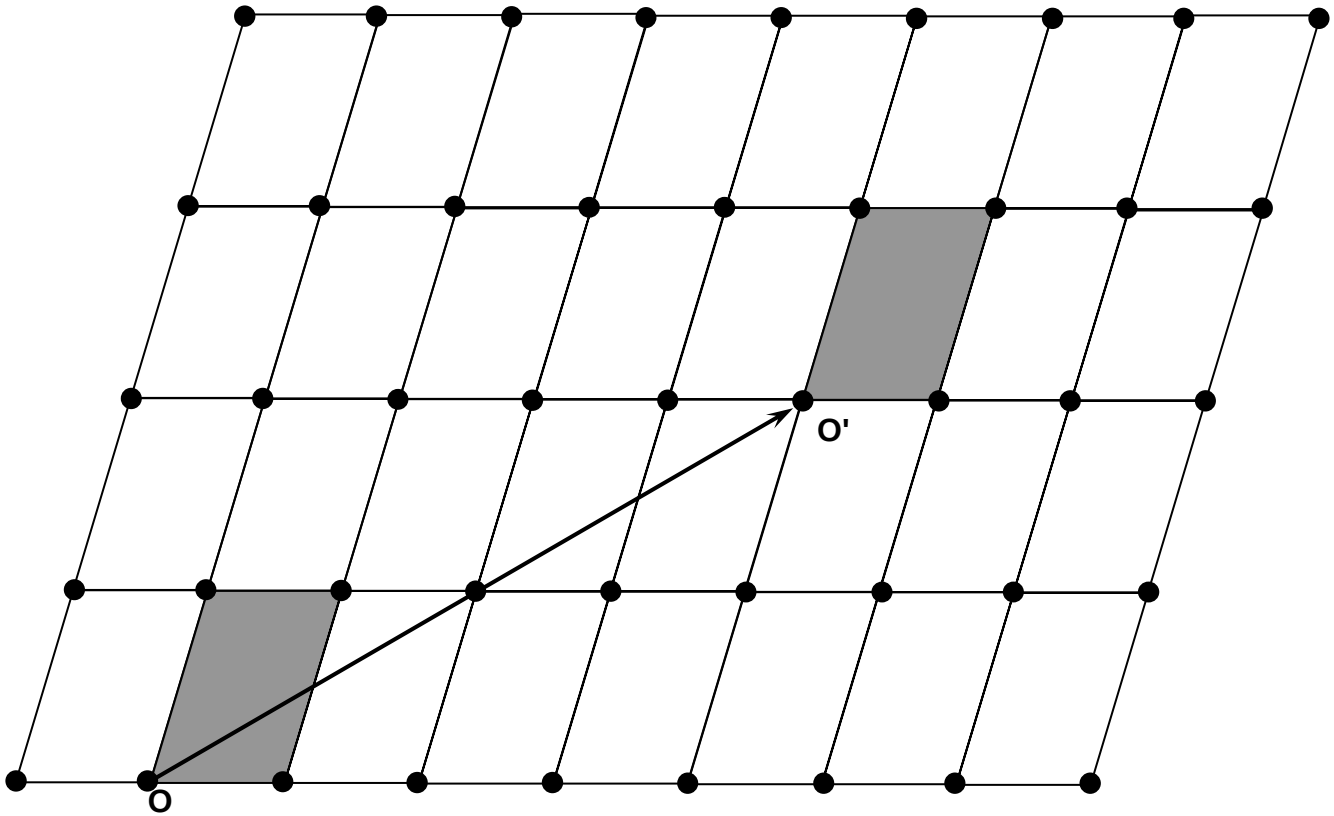
Lattice Structures

- A LATTICE represents a set of points in space that form a periodic structure. Each point sees exactly the same environment. The lattice is by itself a mathematical abstraction.
- A building block of atoms called the BASIS is then attached to each lattice point yielding the crystal structure.

- *LATTICE + BASIS = CRYSTAL STRUCTURE*

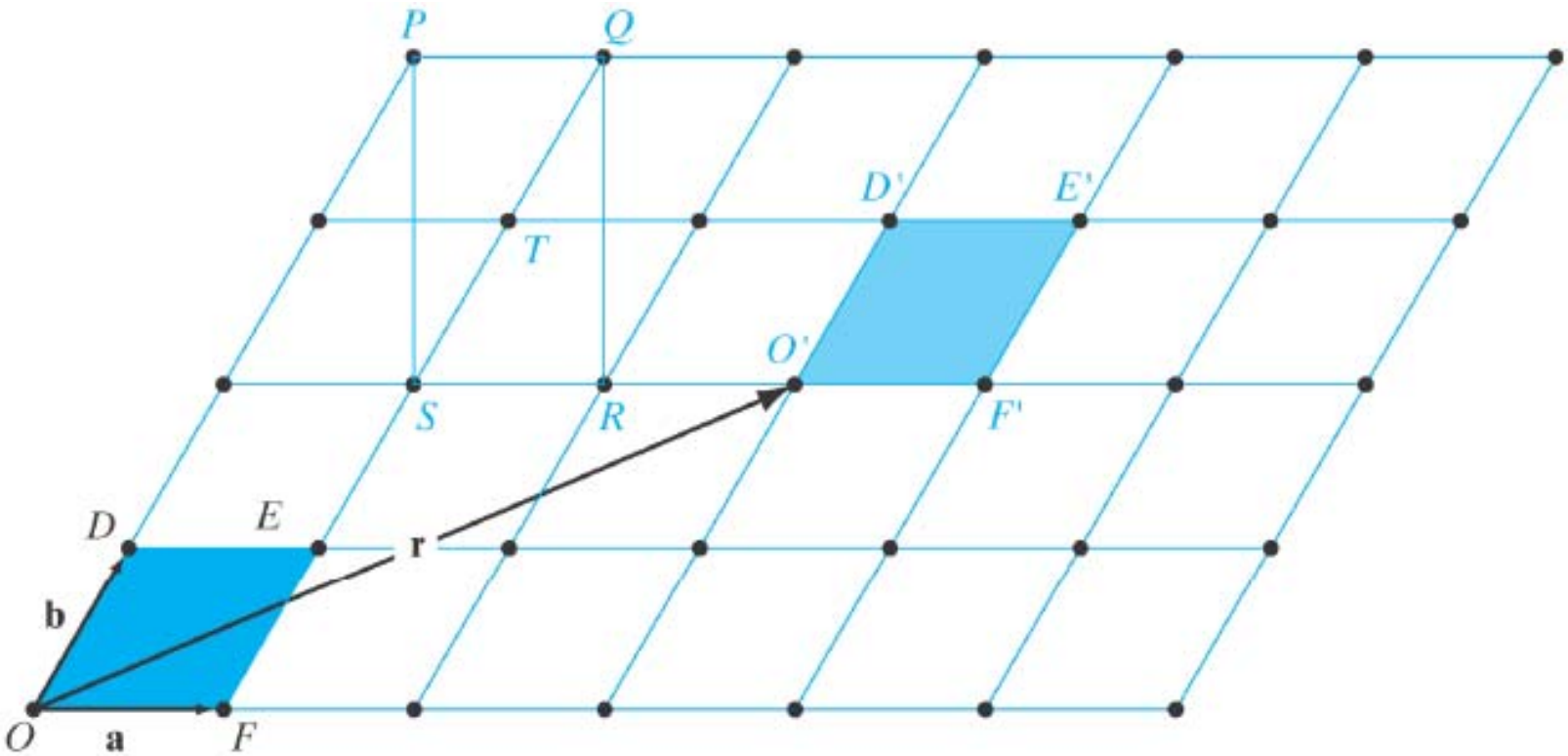
- The identical structure units that have small volume are called UNIT CELL.

Crystal lattices



A 2-D lattice showing translation of a unit cell by R = 4a + 2b

Lattice Structure



ODEF is primitive unit cell and PQRS is the conventional unit cell of the above lattice

Crystals

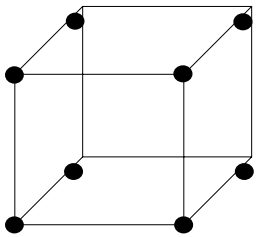
The smallest unit cell is called PRIMITIVE CELL and the cell that is most convenient to study crystal structure is called CONVENTIONAL UNIT CELL.

A unit cell contains all the structural and physical properties of the crystal.

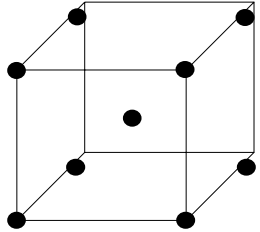
A unit cell IS NOT a unique entity.

The relationship between unit cell and lattice is characterized by three vectors, . Every equivalent lattice point in the 3-D crystal can be found using the vector:

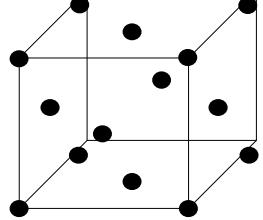
R = pa +qb + sc **,** ***p, q, s*** **are integers.**



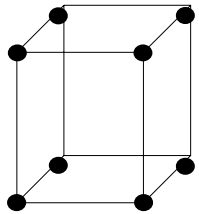
Cubic *P*



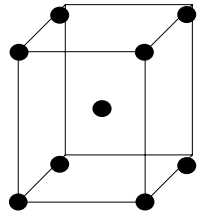
Cubic *I*



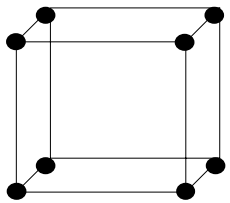
Cubic *F*



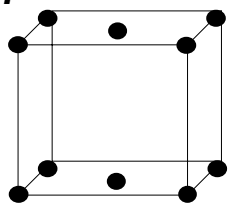
Tetragonal *P*



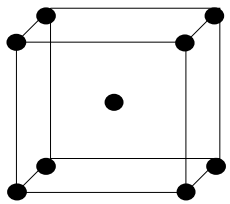
Tetragonal *I*



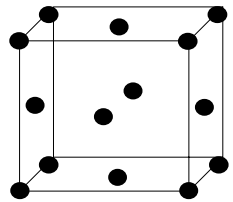
Orthorhombic *P*



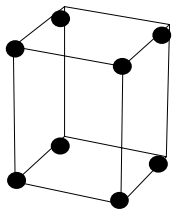
Orthorhombic *C*



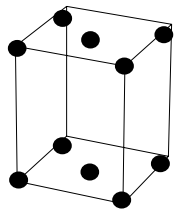
Orthorhombic *I*



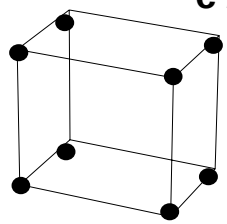
Orthorhombic *F*



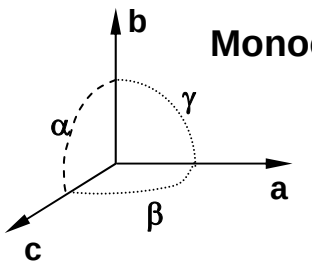
Monoclinic *P*

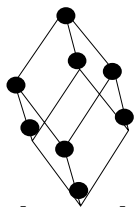


Monoclinic *C*

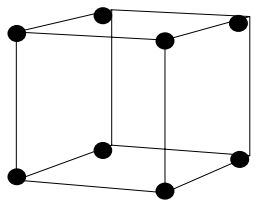


Triclinic



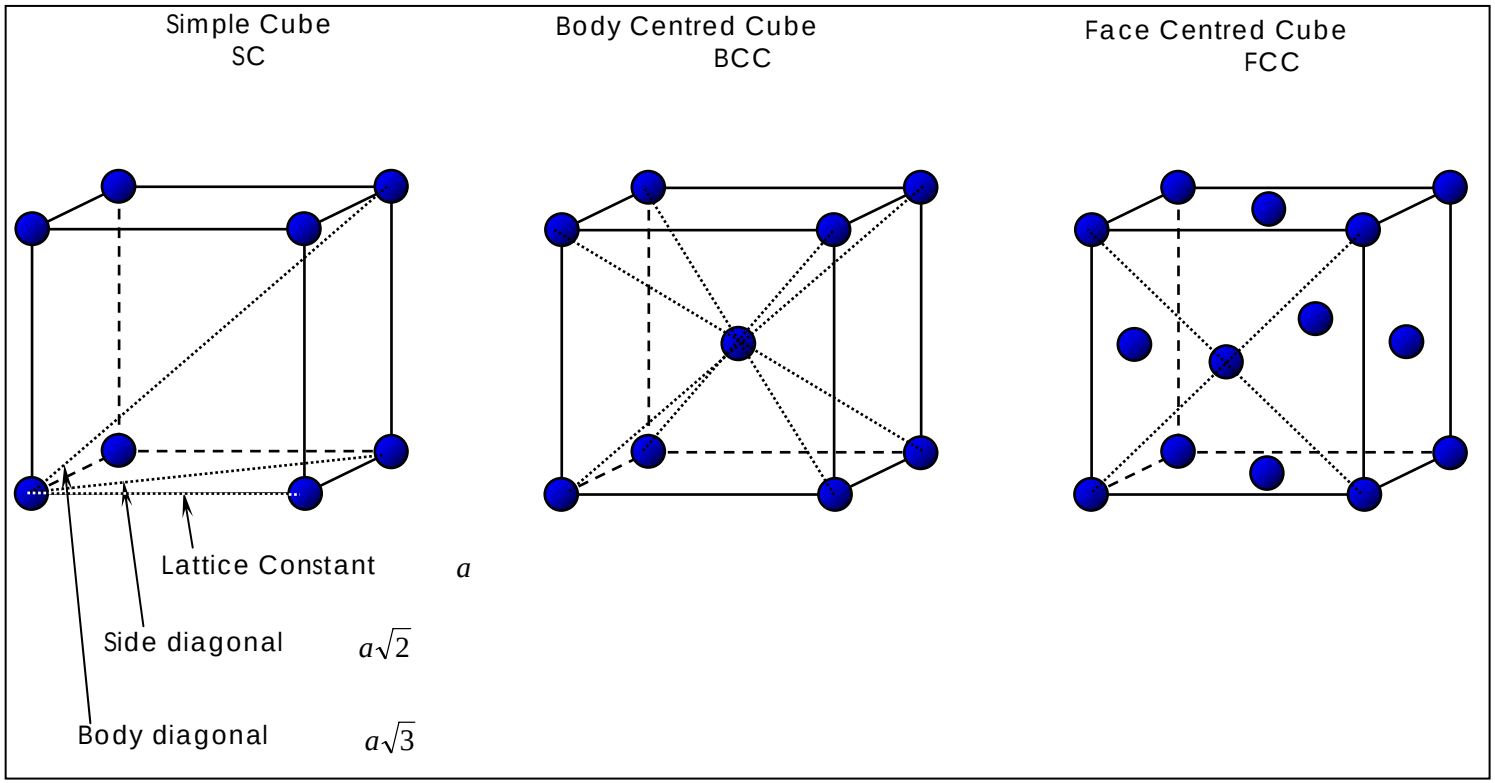


Trigonal *R*

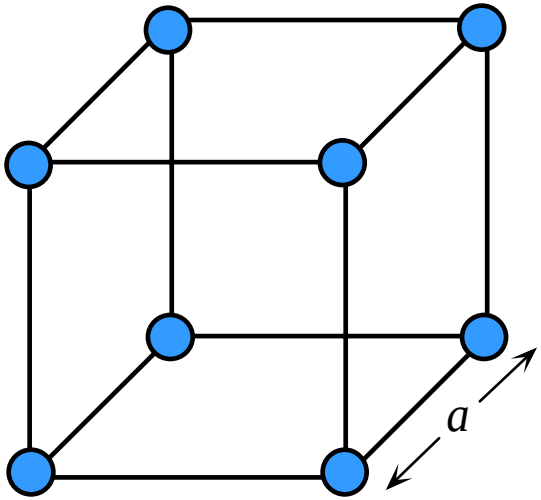


Trigonal and Hexagonal *R*

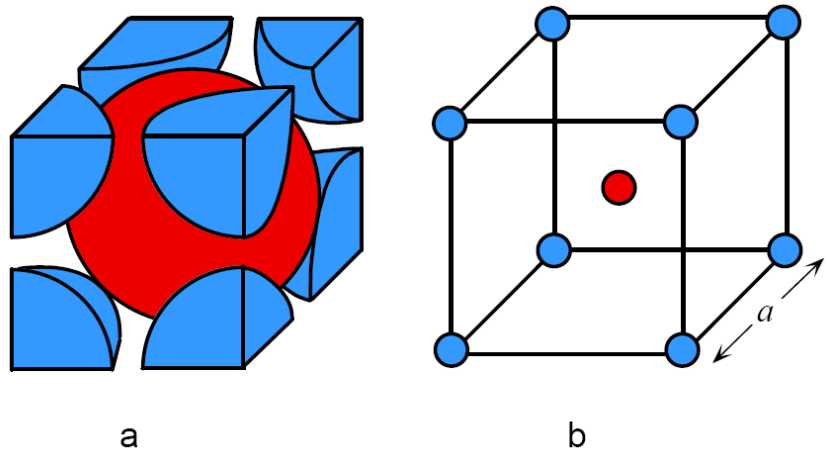
Lattice Structures



Examples of SC & BCC



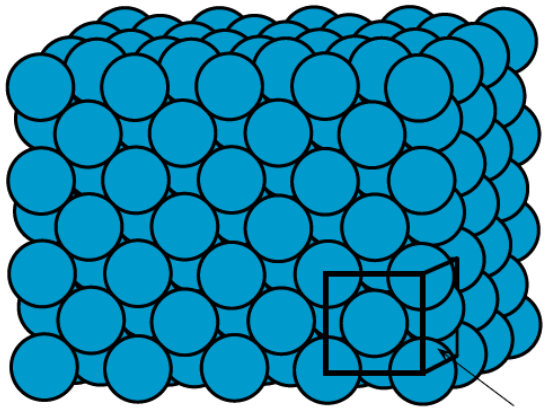
Simple cubic (SC): Polonium (Po)



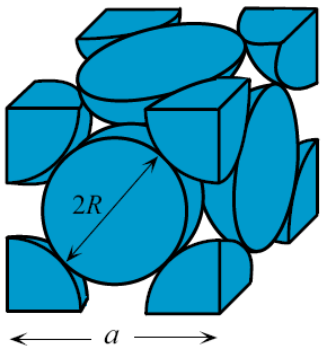
Body centered cubic **(**BCC) unit cell: Alkali metals (Li, Na, K), Cr, Mo, Mn

Ref: S.O. Kasap, Principles of Electronic materials and devices

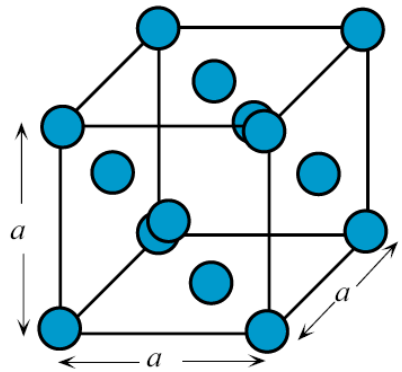
Example of FCC Structure



(a)



(b)



(c)

(a) The crystal structure of copper is face centered cubic (FCC). The atoms are positioned at well defined sites arranged periodically and there is a long range order in the crystal.

(b) An FCC unit cell with closed packed spheres.

(c) Reduced sphere representation of the unit cell. Examples: Ag, Al, Au, Ca, Cu, Ni.

Number of atoms per unit cell

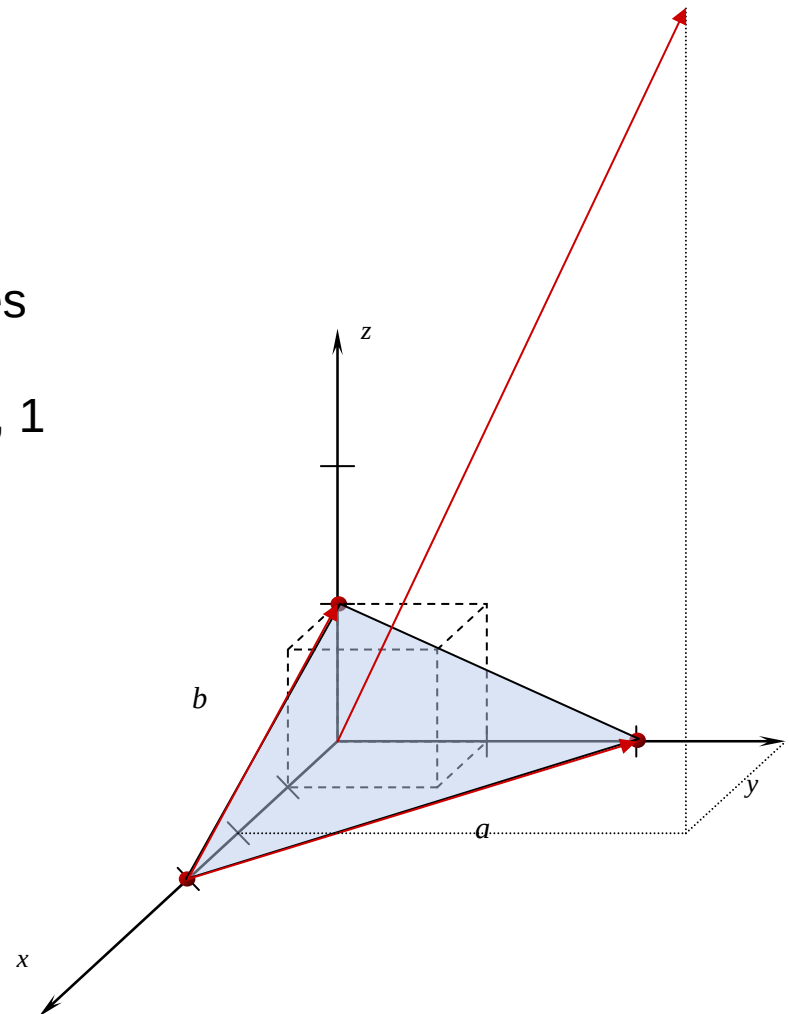
8 corners = 8 × (1/8)=1

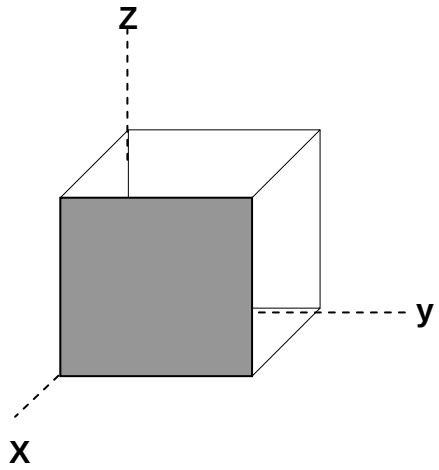
6 faces = 6 × (1/2) = 3

Lattice Structure

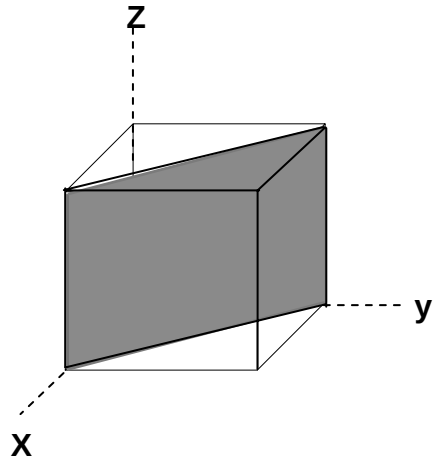
- Miller Indices

For any cubic unit cell system:
- build axes along the edges of unit cell
- normalize intercepts: 3, 2, 1
- invert intercepts: 1/3, 1/2, 1
- adjust: 2/6, 3/6, 6/6
- Miller Indices: (236)

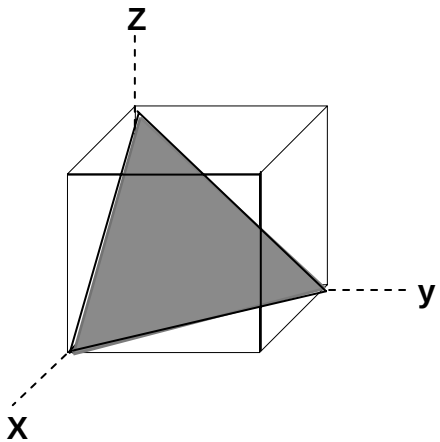




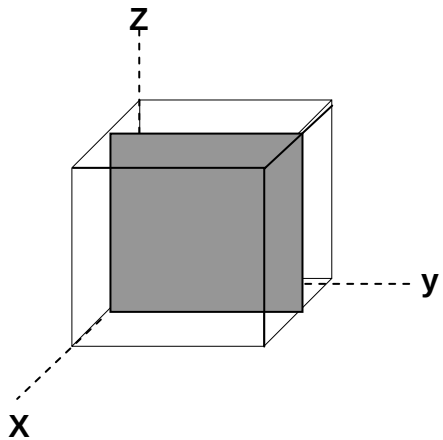
(100)



(110)



(111)



(200)

Some popular lattice planes

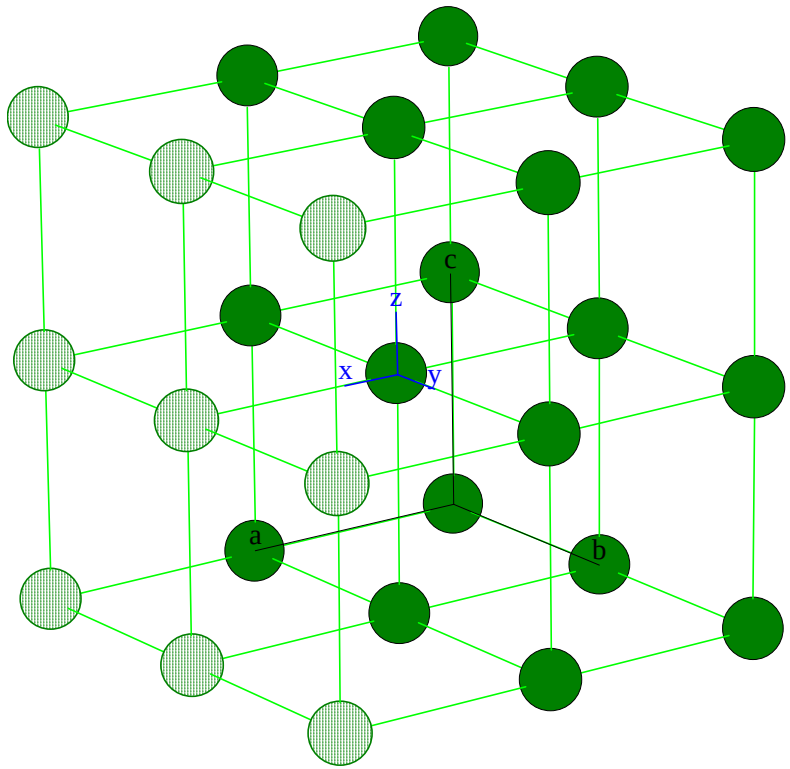
Crystals

Parameters that characterize a crystal structure:

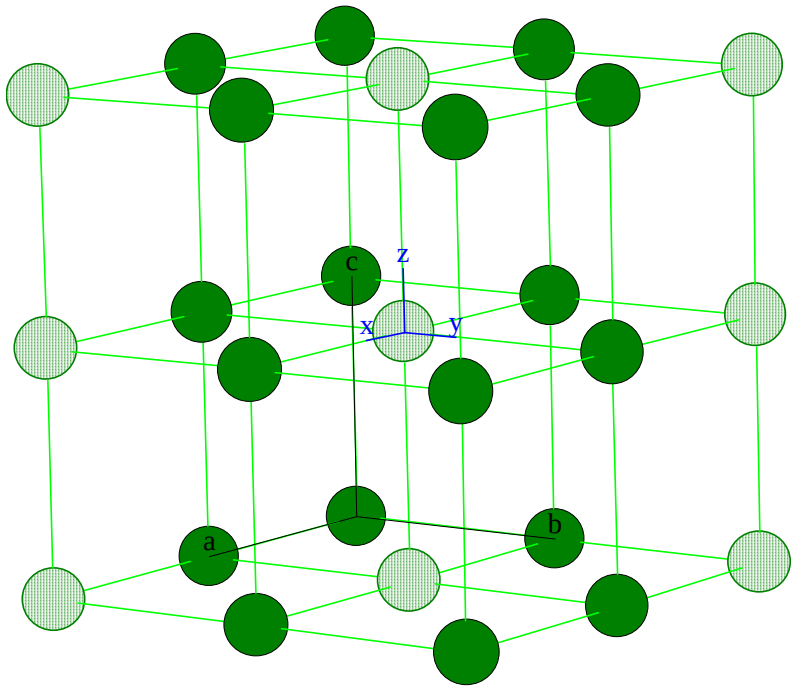
- Lattice structure (e.g. cubic, tetragonal, etc.).
- Basis.
- Number of atoms in a unit cell.
- Crystal planes e.g. {100}, {110}, {111}, Miller Indices.
- Number of atoms in each plane.
- Chemical binding (e.g. metallic, covalent, …).
- Number of nearest (nn) and next nearest (nnn) atoms to each atom.

Example of (100)

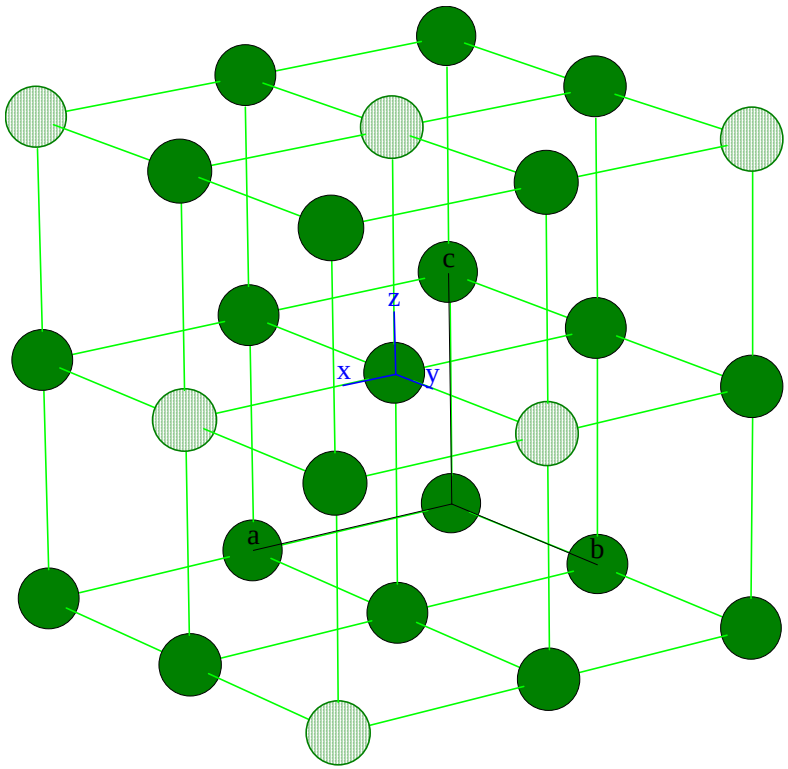
(100)



Example of (110)

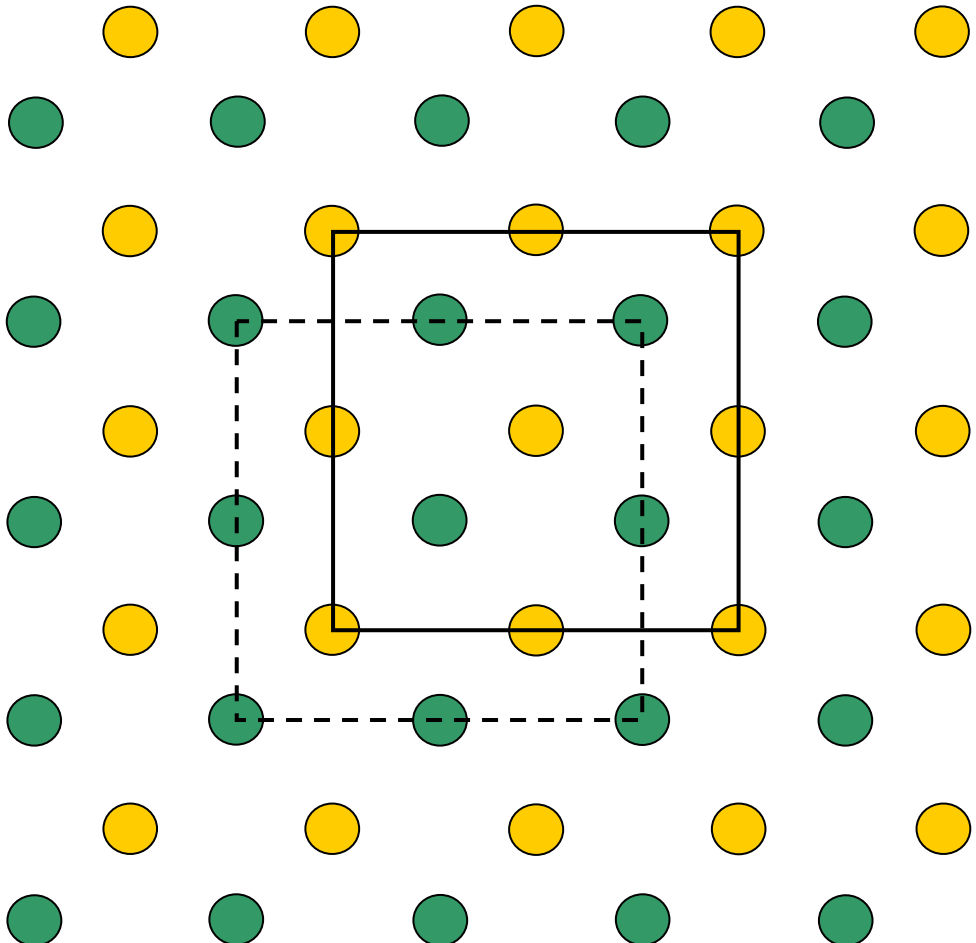


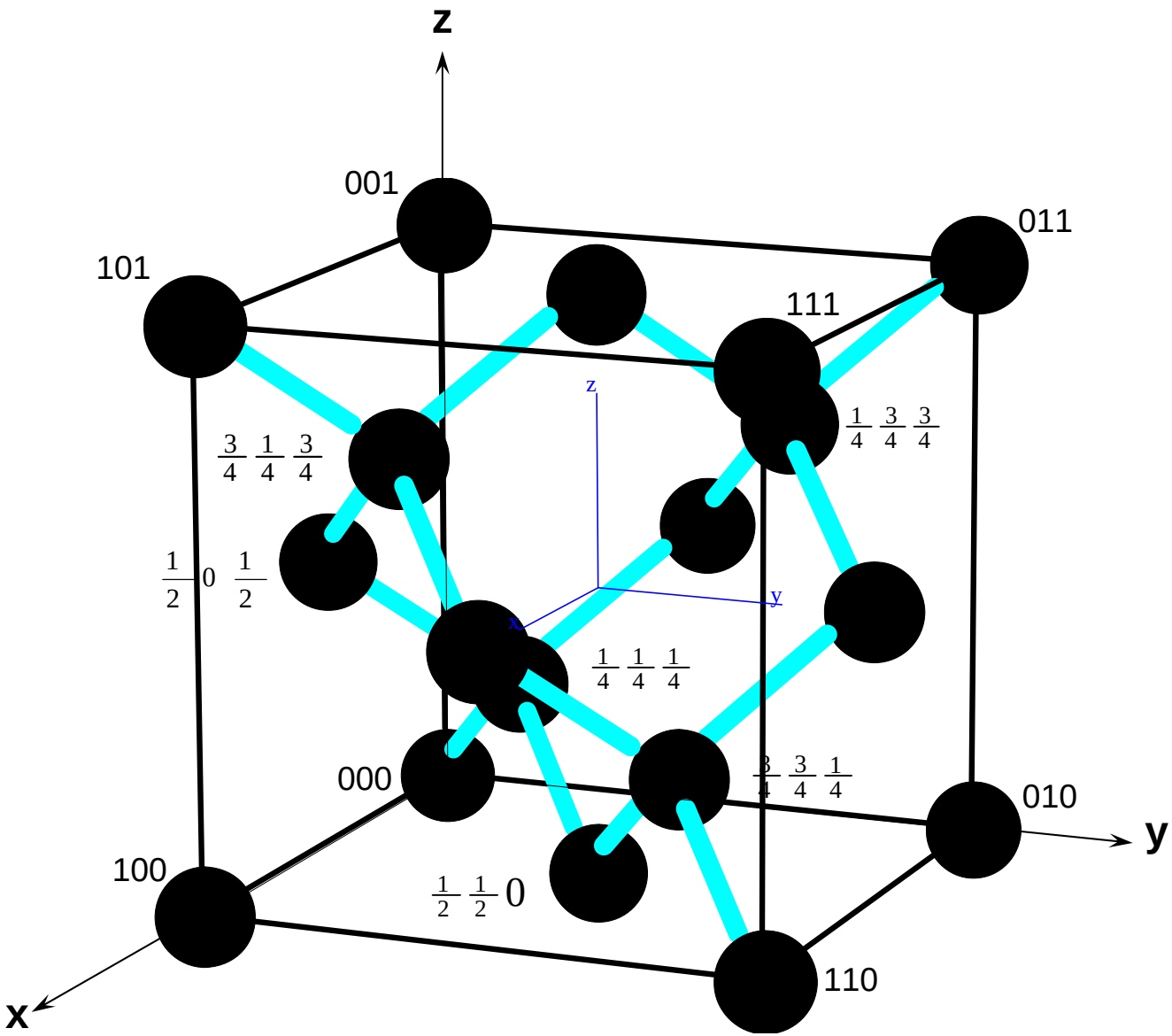
Example of (111)



Diamond Structure

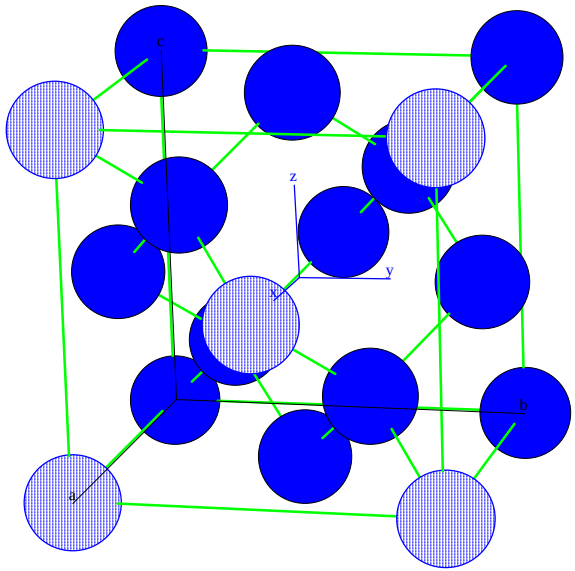
- Top view of an extended (100) plane of the diamond lattice structure.



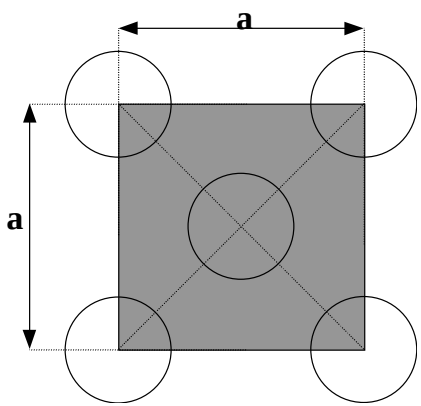


The unit cell of diamond lattice structure. The position of each lattice point is shown with respect to the 000 lattice point.

Si (100) Crystal

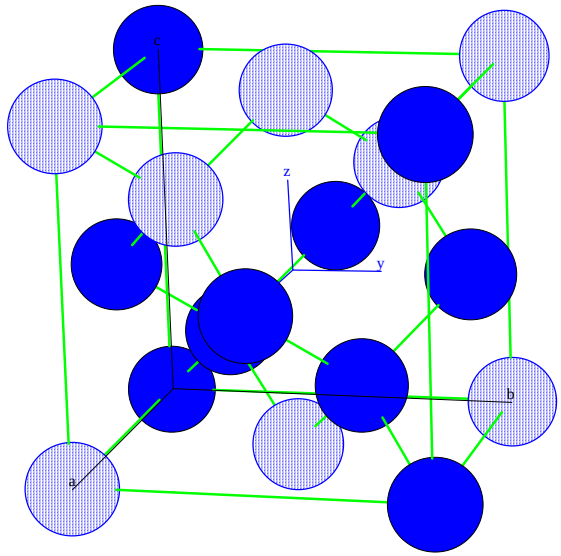


- Plane intercepts at x=1

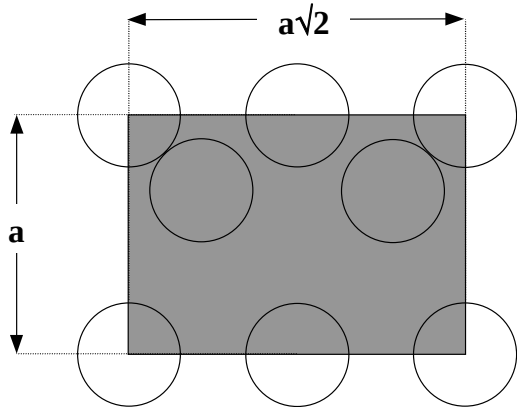


- Plane contains 2 unit cells (1+¼+¼+¼+¼)

Si (110) Crystal

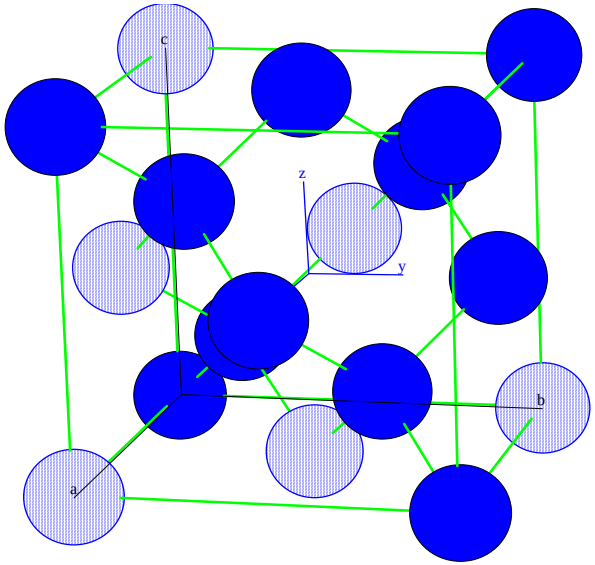


- Plane intercepts at
  x=1, y=1

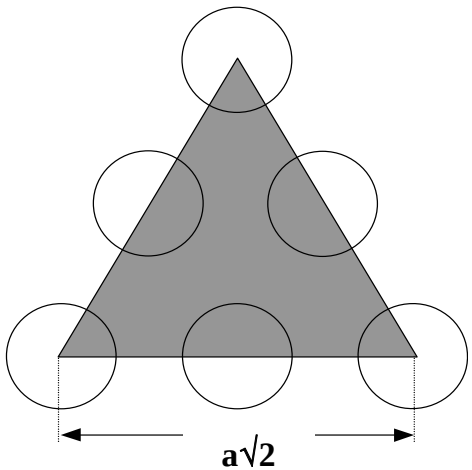


- Plane contains 4 unit cells (2 + 2*½ + 4*¼)

Si (111) Crystal

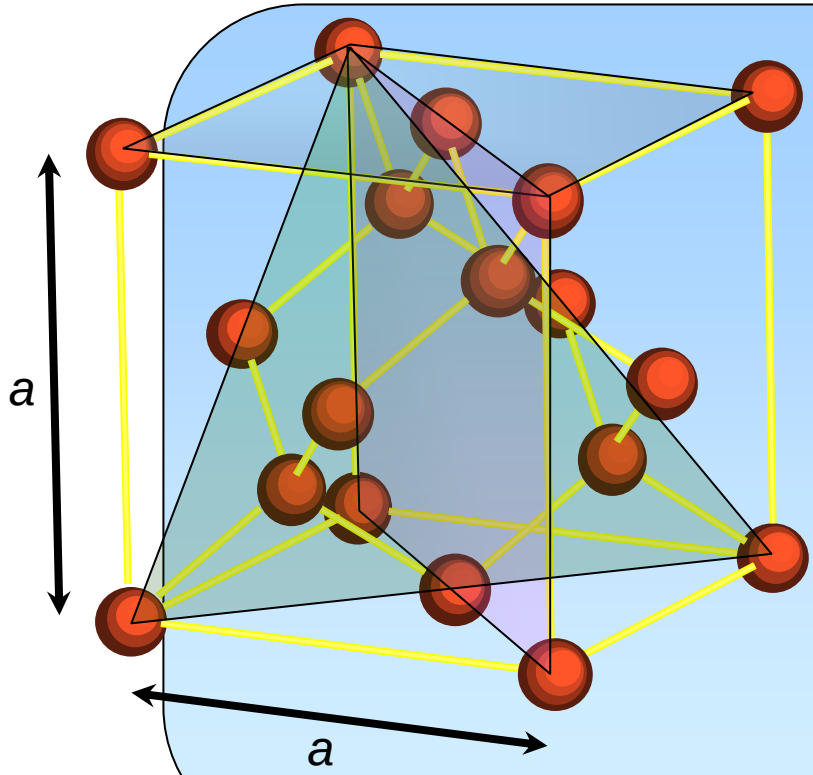


- Plane intercepts at x=1, y=1, z=1



- Plane contains 2 unit cells (3*½ + 3*1/6)

Two Interpenetrating Face-Centered Cubic Lattices
Silicon – Diamond Structure

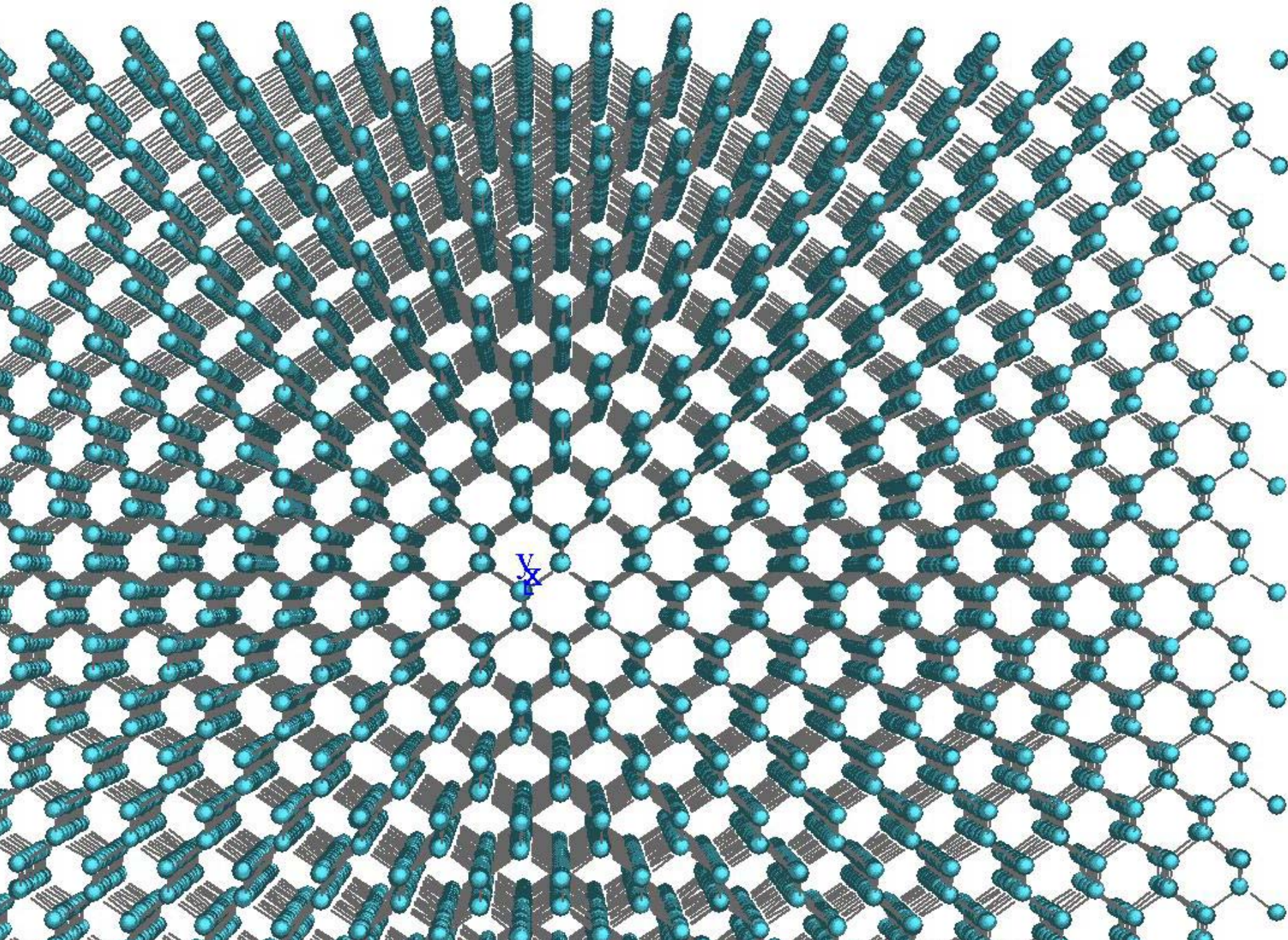


Common Planes

- {100} Plane
- {110} Plane
- {111} Plane

a – Lattice Constant
For Silicon

$a = 5.34$ Å


Y
X

Terms used often to characterize a crystalline structure:

1) Relationship between lattice constant and radius of the atoms

2) Atomic packing factor (APF) defined as:

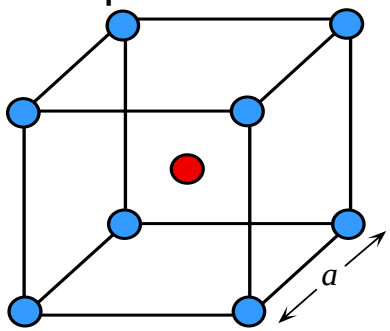
$$\text{APF} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$$

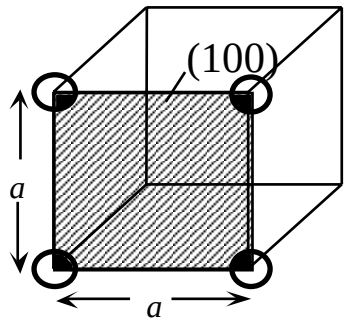
3) Atomic surface density (# of atoms/unit of area) and volume density (# of atoms /unit of volume)

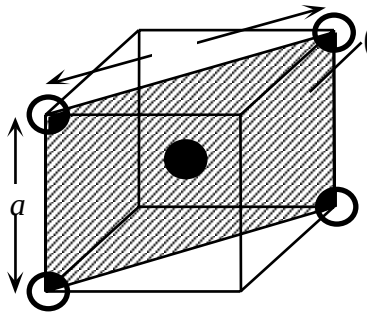
4) Distance between nearest neighboring atoms

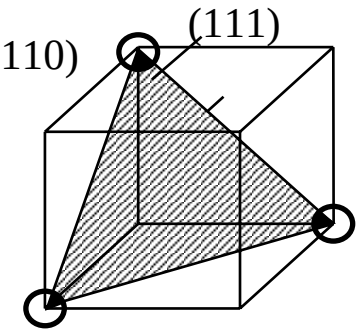
Example 1.3. Consider a BCC structure.

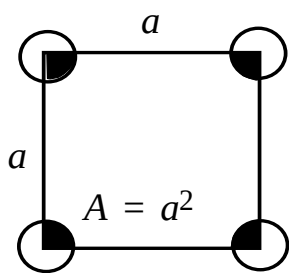
What are the surface density of atoms for (100), (110) and (111) planes?

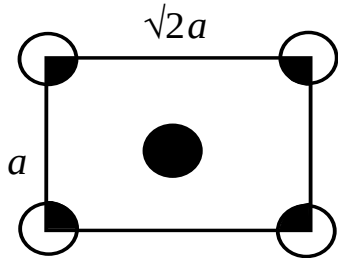


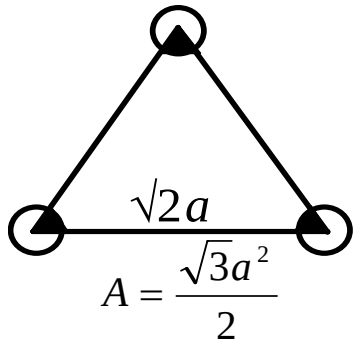












Answers: (100) $\frac{1}{a^2}$ (110) $\frac{2}{\sqrt{2}a^2}$ (111) $\frac{1}{\sqrt{3}a^2}$

Practice: You do this for an FCC structure.

Silicon Production

$$SiC(solid) + SiO_2(solid) \xrightarrow{1600-1800^\circ C} Si(liquid) + SiO(gas) + CO(gas)$$

- Produced silicon at this stage is 98% pure and is called Metallurgical Grade Silicon (MGS).
- For electronic purposes very high pure silicon - Electronic Grade Silicon (EGS) is needed.
- To obtain EGS from MGS the following reactions are used:

$$Si(solid) + 3HCl(gas) \xrightarrow{300^\circ C} SiHCl_3(gas) + H_2 + heat$$

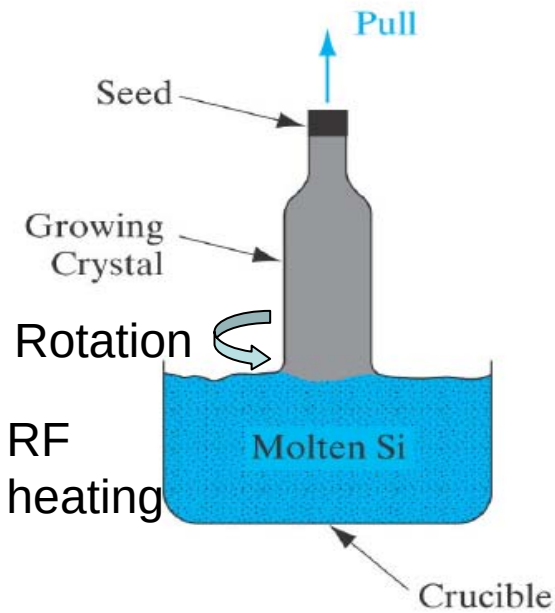
$$2SiHCl_3(gas) + 2H_2(gas) \rightarrow 2Si(solid) + 6HCl(gas)$$

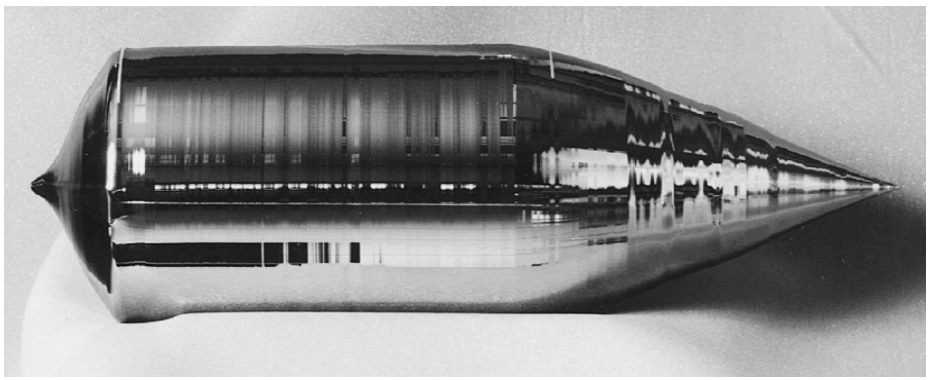
The above process is called chemical vapour deposition (CVD) and the produced Si is polycrystalline and 99.999% pure.

Silicon crystal preparation

Single crystal Ingots or boules (bulk):

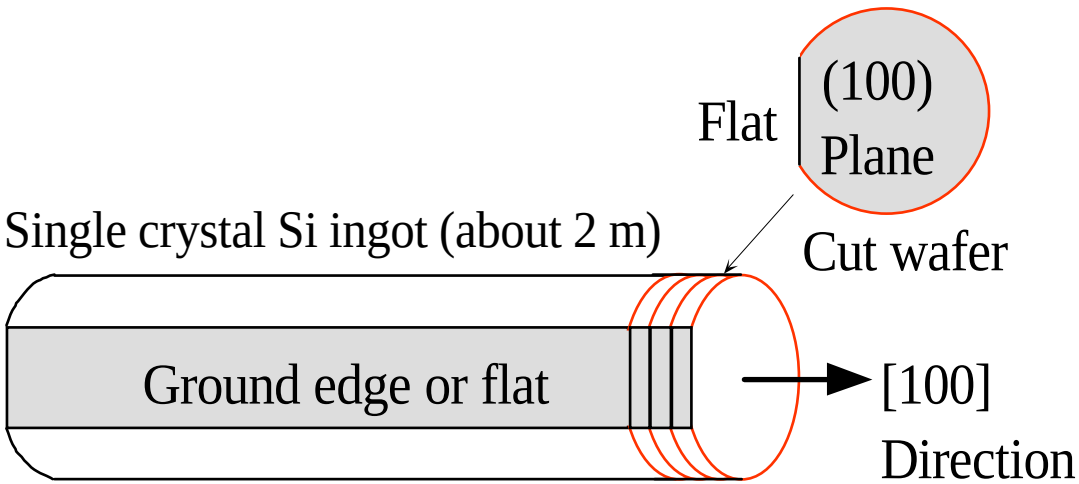
A large single crystal Ingot grows from melt polycrystalline Si, using solidification on a seed crystal. The seed is slowly pulled from the melt. As the seed is slowly pulled, solidification occurs along the plane between the solid-liquid interface. Usually the crystal is also rotated slowly to provide a slight stirring action to the melt, resulting a more uniform temperature.





Single crystal: 20-30 cm in diameter and 1-2 m in length.

Silicon wafers production



Silicon Wafer

- Type
  - n-type (e.g.,As,P, Bi doping)
  - P-type (B, Ga, In dopin
- Orientation
  - {100}, {111},...