ECE 340: Semiconductor Electronics

Chapter 1: Crystal Properties and Growth of Semiconductors

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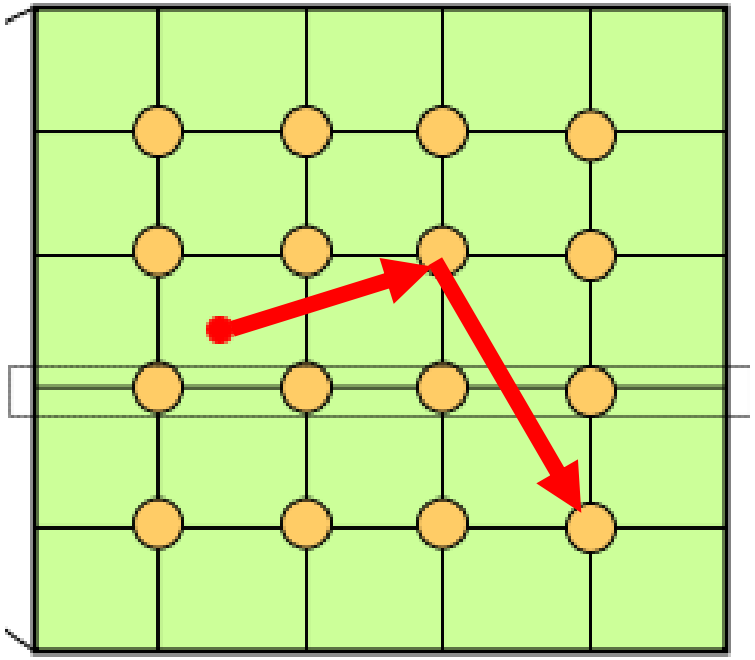
Why do we need to study crystal structure?

- Because the transport of charge through a metal or semiconductor depends on the arrangement of atoms in the solid



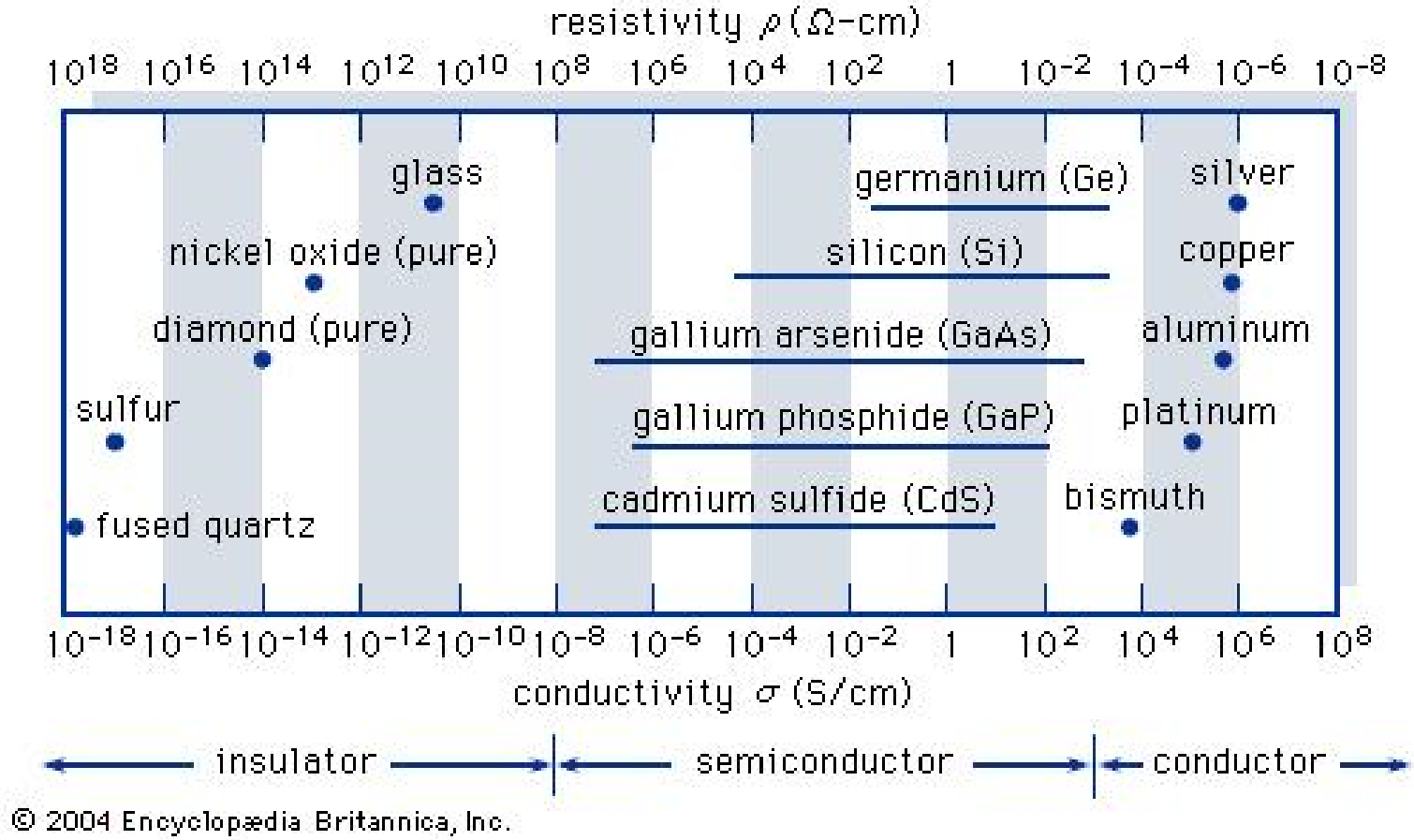
Material types by electrical resistivity

- Insulators: very high resistivity
  - Diamond (SiO2)
  - Electric Resistivity = 1018 Ω m

- Metals: very low resistivity
  - Gold (Au)
  - Electric Resistivity = 22.14 nΩ m

- Semiconductors: intermediate resistivity
  - Silicon (Si)
  - Electric Resistivity = 103 Ω m

- Where semiconductors fit in (electrically):



Semiconductor material

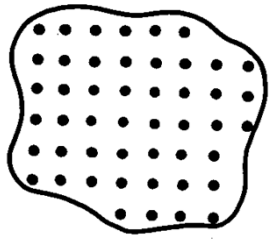
Table 1–1 Common semiconductor materials: (a) the portion of the periodic table where semiconductors occur; (b) elemental and compound semiconductors.

(a)	II	III	IV	V	VI
		B	C	N	
		Al	Si	P	S
	Zn	Ga	Ge	As	Se
	Cd	In		Sb	Te

(b)	Elemental	IV compounds	Binary III–V compounds	Binary II–VI compounds
	Si	SiC	AlP	ZnS
	Ge	SiGe	AlAs	ZnSe
			AlSb	ZnTe
			GaN	CdS
			GaP	CdSe
			GaAs	CdTe
			GaSb	
			InP	
			InAs	
			InSb	

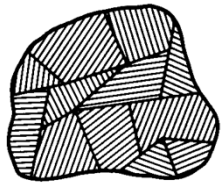
Structure types in solid material

- **Crystalline:** atoms are ordered into a well-defined lattice that extends over very long distances;



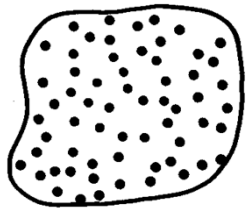
crystalline

- **Polycrystalline:** consist of many small regions of single-crystal material;



polycrystalline

- **Amorphous:** no periodic structure;



amorphous

Primitive Cell and Unit Cell

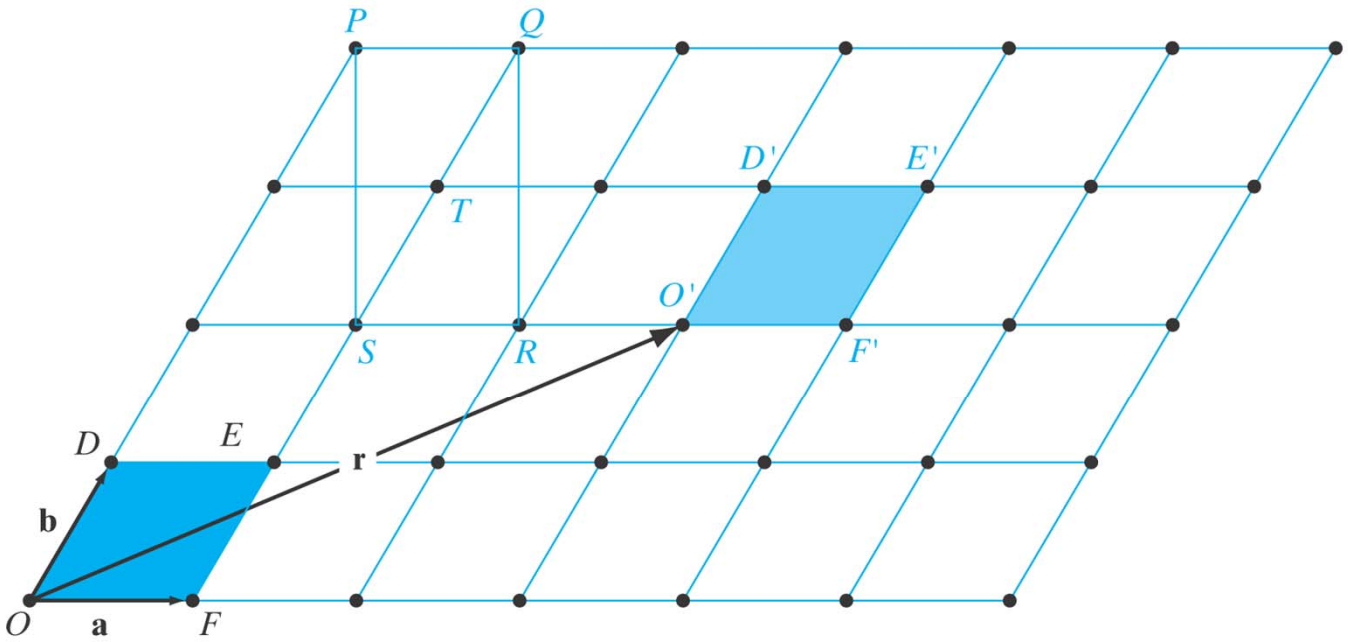
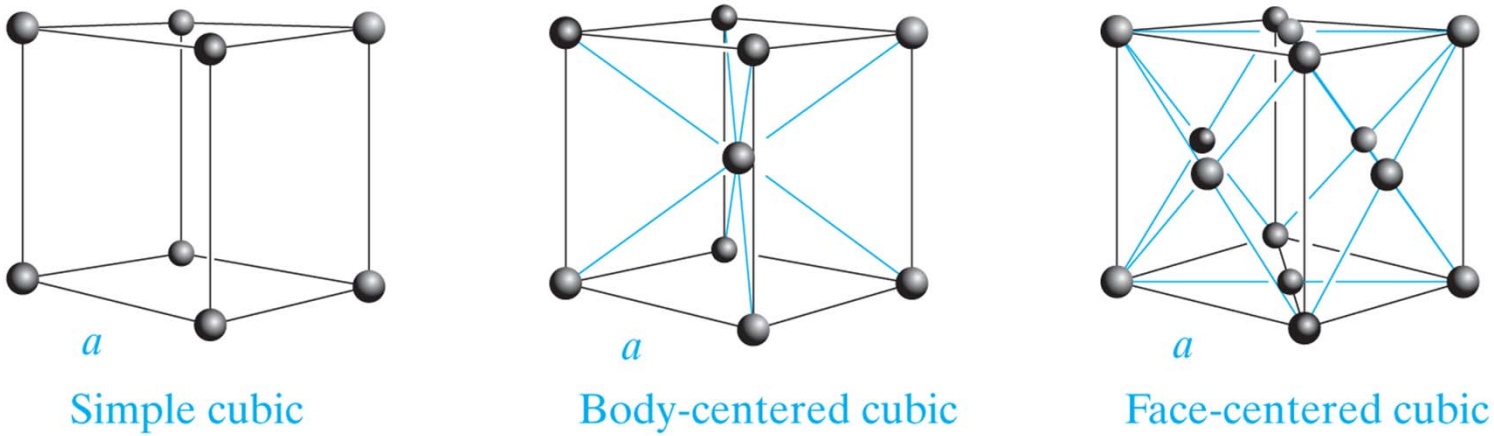


Figure 1.2

A two-dimensional lattice showing translation of a unit cell by $\mathbf{r} = 3\mathbf{a} + 2\mathbf{b}$.

- Primitive cell: smallest cell, ODEF.
  Unit cells: allowing center lattice points, PQRS with center T

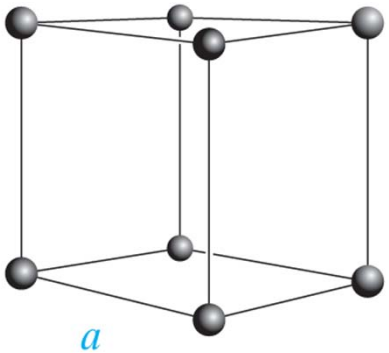
Unit Cell - Cubic Lattice



a is called lattice constant.

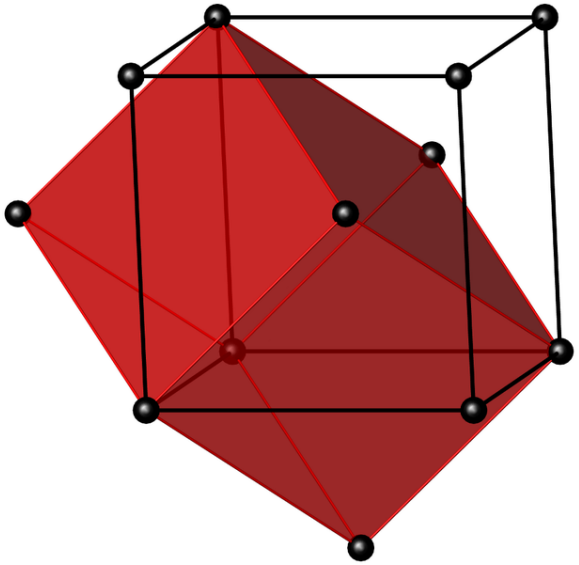
Primitive cell

Simply cubic

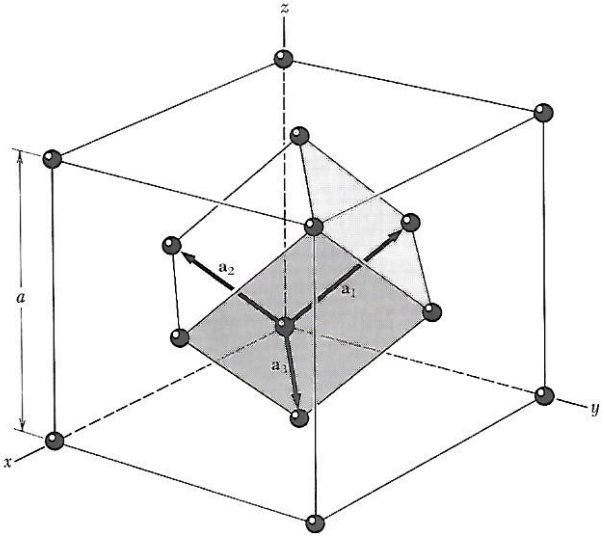


Simple cubic

Body-centered cubic

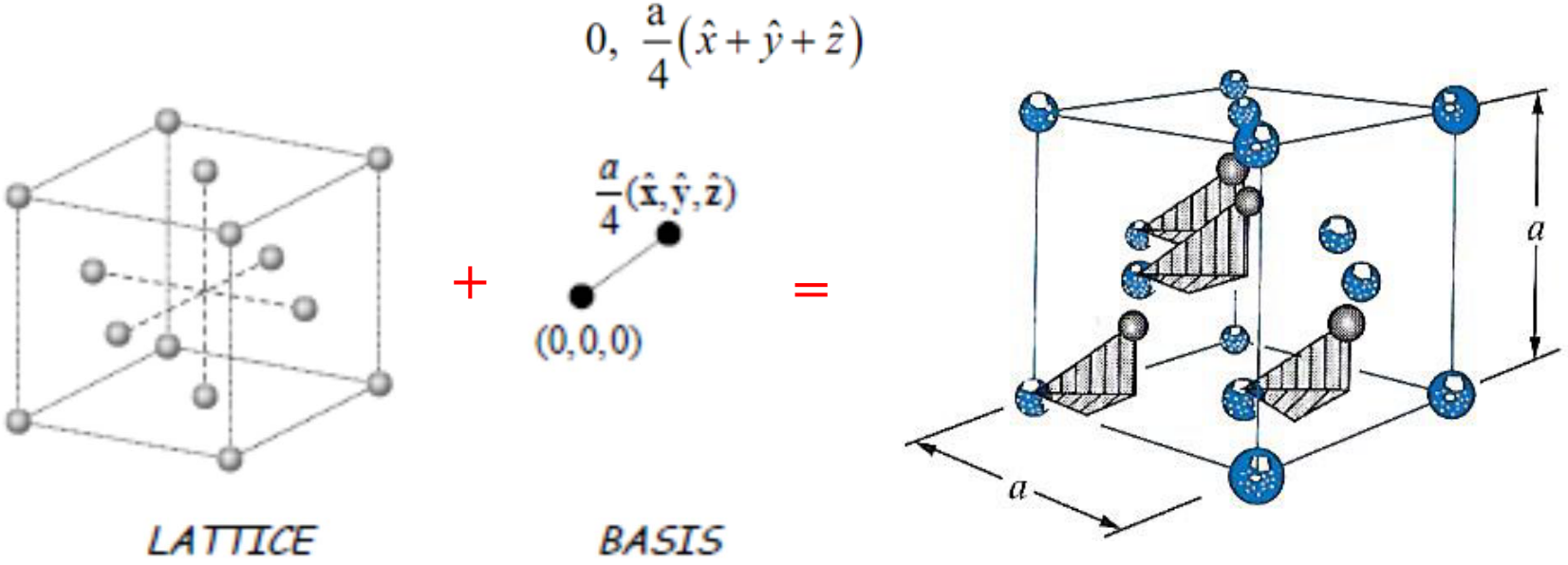


Face-centered cubic

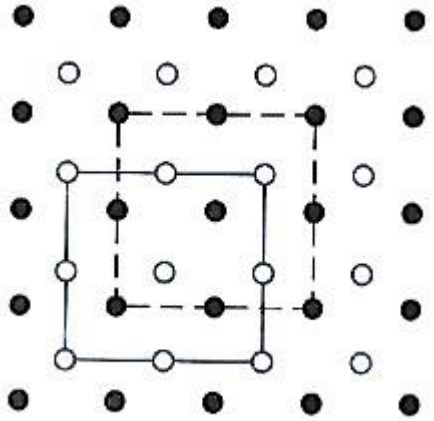


Diamond Lattice

- Diamond structure can be described as an FCC lattice with a 2 atom basis.

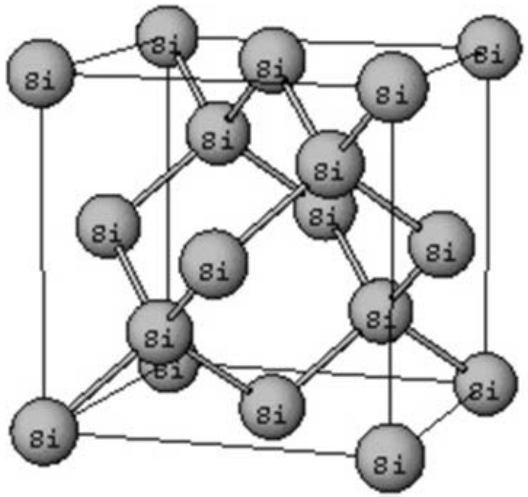


- 2 atom basis to a FCC lattice
- Tetrahedral bond arrangement
- Each atom has 4 nearest neighbors
- Elements crystallizing in the diamond structure are: C, Si, Ge



Top view

Diamond Lattice vs. Zinc Blende



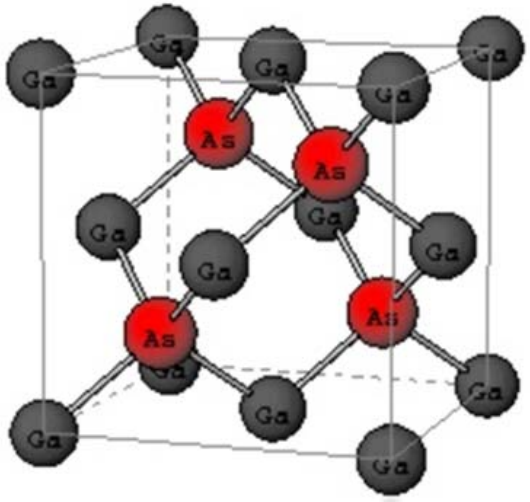
Silicon

Diamond Cubic Structure

4 atoms at (0,0,0)+ FCC translations

4 atoms at (¼,¼,¼)+FCC translations

Bonding: covalent



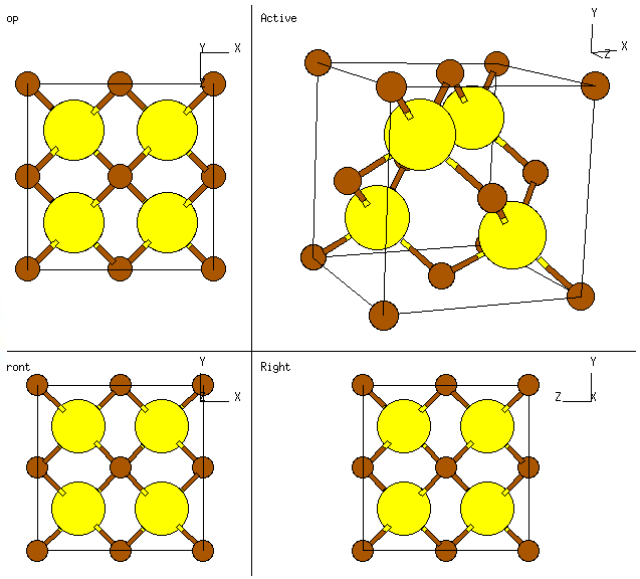
GaAs

ZnS (Zinc Blende) Structure

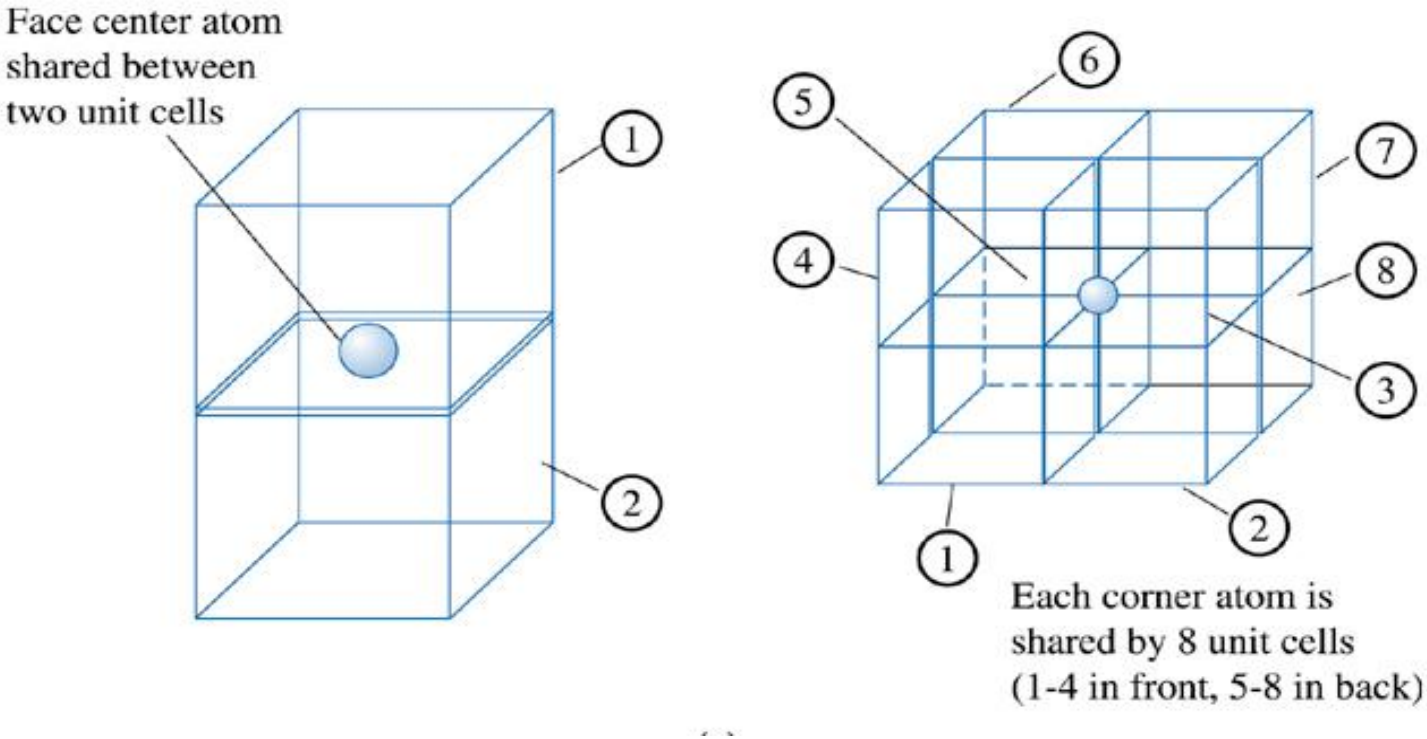
4 Ga atoms at (0,0,0)+ FCC translations

4 As atoms at (¼,¼,¼)+FCC translations

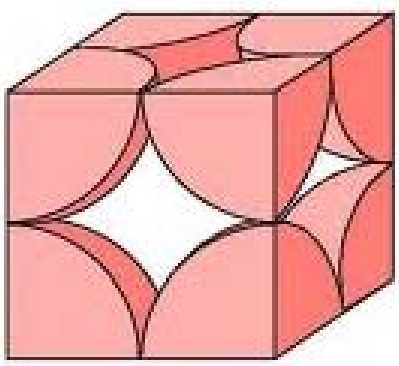
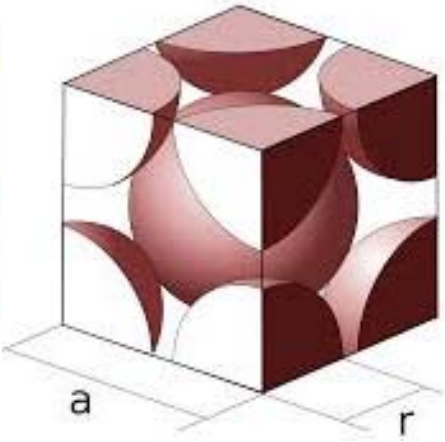
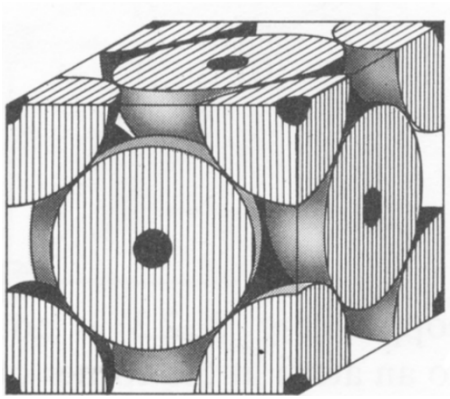
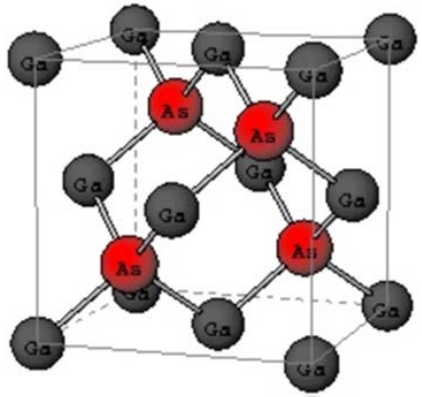
Bonding: covalent, partially ionic



Number of Atoms per Unit Cell

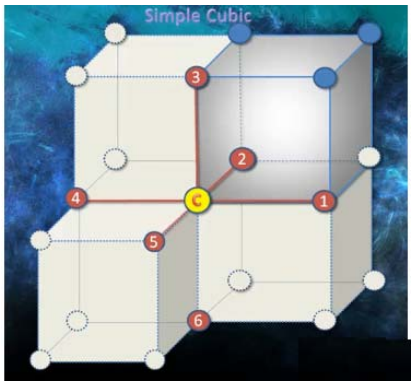


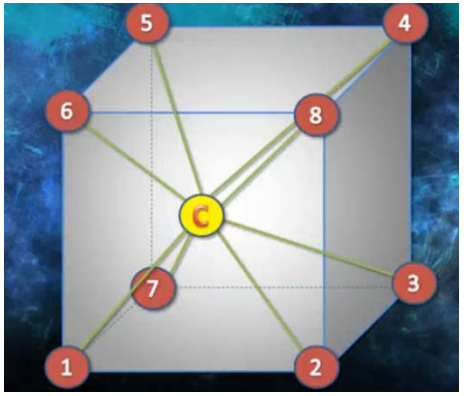
Number of Atoms per Unit Cell

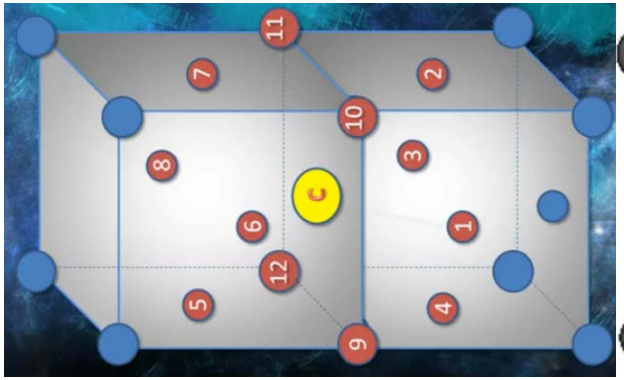
SC	BCC	FCC	Diamond or Zinc Blende
			
# of atoms per unit cell:	**1**	—	—	—

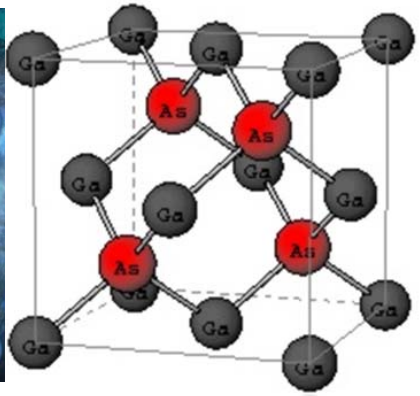
Nearest Neighbor

SC **BCC** **FCC** **Diamond or Zinc Blende**









# of nearest neighbor:

	6		
nearest neighbor distance:			
	a		

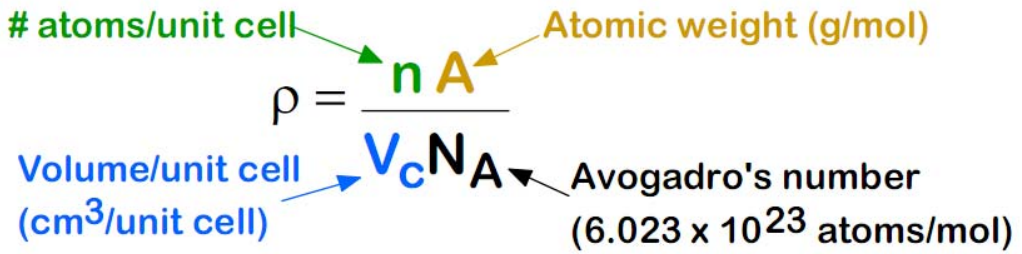
Density Calculations:

ATOMIC DENSITY: Number of Atoms per Unit Volume

$$\frac{\#\ \text{atoms}}{\text{cm}^3} = \frac{n}{V_C} = \frac{\#\ \text{atoms/unit cell}}{\text{Volume/unit cell}}$$

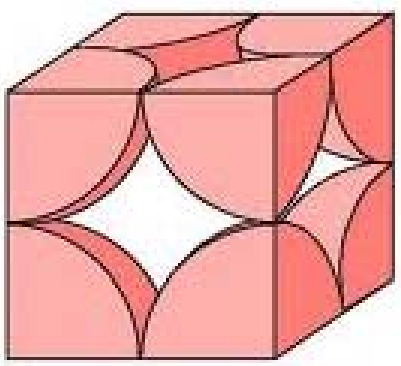
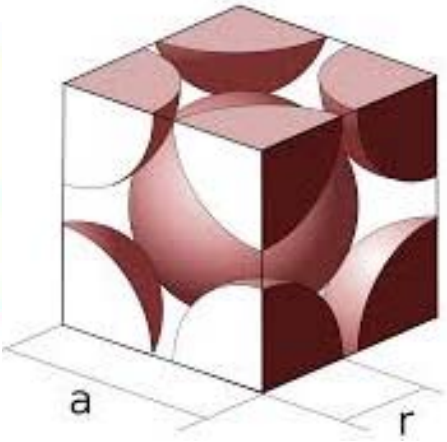
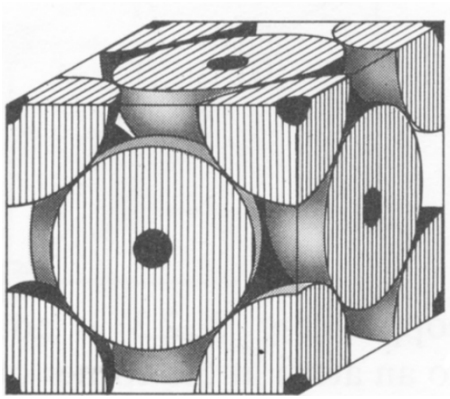
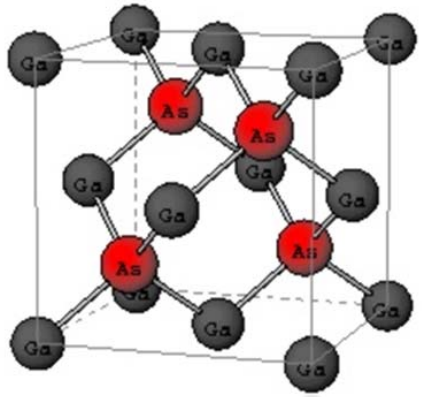
MASS DENSITY: ρ = $\dfrac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$

Theoretical Density



Avogadro constant is defined as the number of constituent particles (usually atoms or molecules) per mole of a given substance

Atomic density

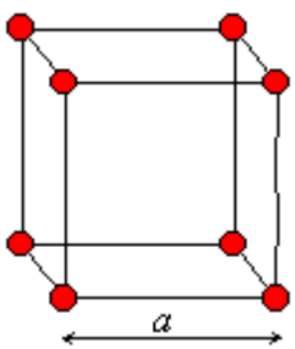
SC	BCC	FCC	Diamond or Zinc Blende
			
Atomic density: $\frac{1}{a^3}$	—	—	—

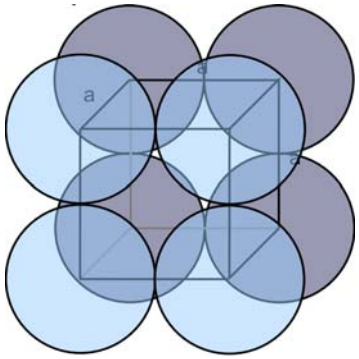
Packing Density Fraction

Packing density fraction, or atomic packing factor (APF), is the fraction of a volume filled with atoms, when atoms are close-packed.

$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}}$$

Simple Cubic Example



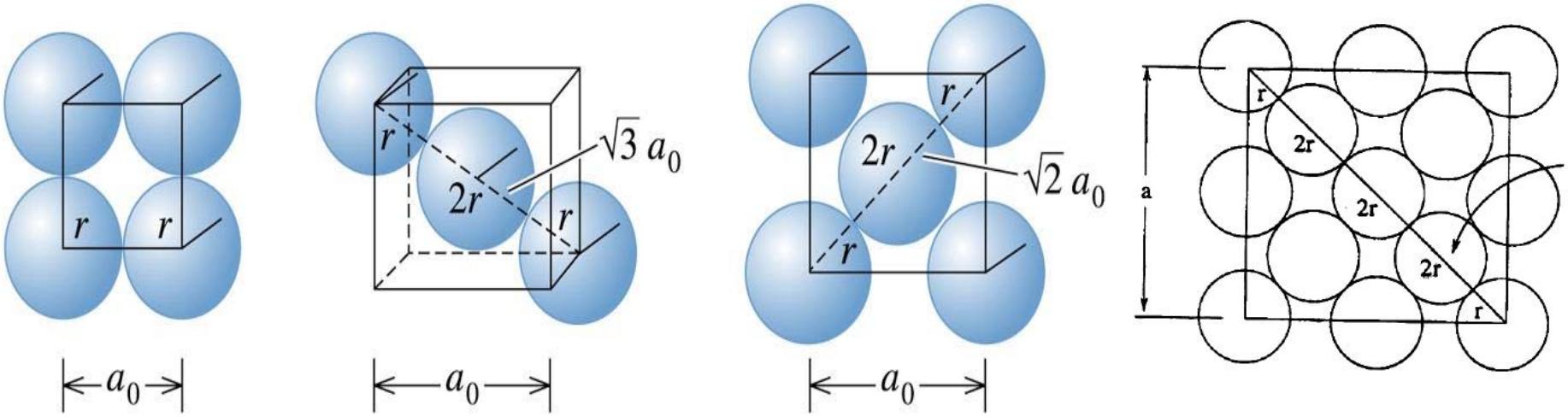


$$\frac{\text{Volume of atoms}}{\text{Volume of the unit cell}} = \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 52\%$$

	Radius	Atoms/ unit cell	Packing Density
Simple Cubic	$\frac{a}{2}$	1	$\frac{\pi}{6} = 52\%$

Maximum radius of the atom and packing density

SC **BCC** **FCC** **Diamond or Zinc Blende**



Maximum radius of the atom:

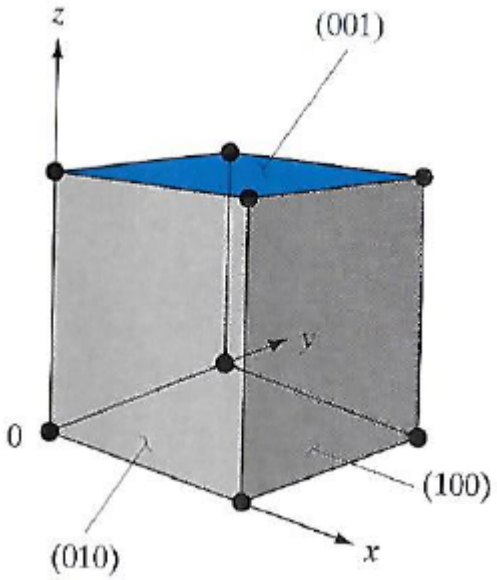
$$r = a_0/2$$

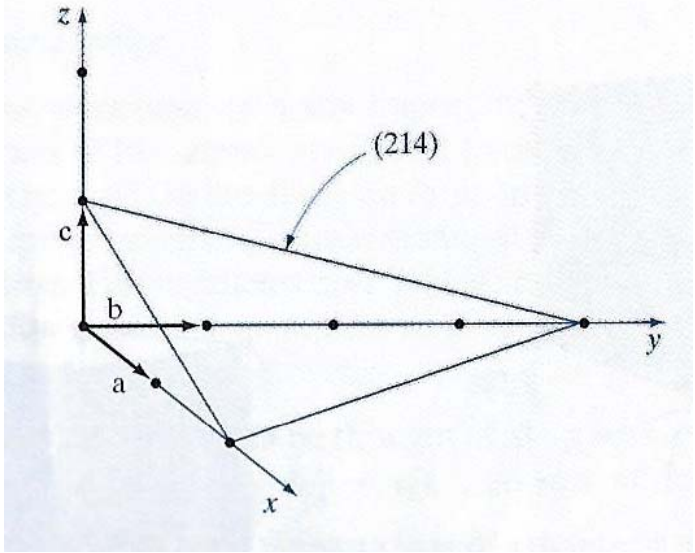
Packing density fraction:

$$\frac{\pi}{6}$$

Miller index of crystal plane

1. Locate the intercepts of the desired plane with the coordinate axes.
2. Take the reciprocal of the intercepts and reduce these to the smallest set of integers *h,k,l*.
3. Label the plane (*hkl*)





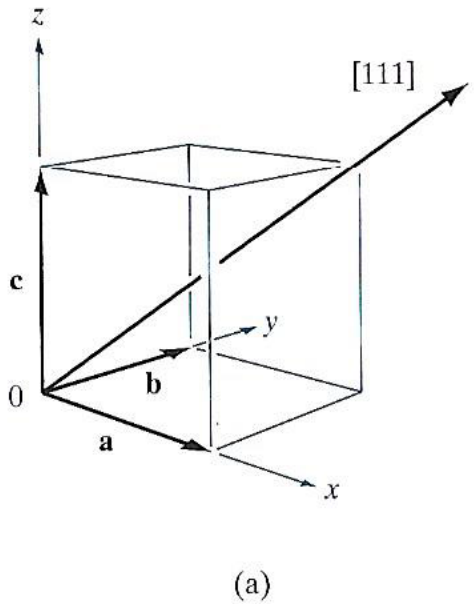
Axis	Intercept	Reciprocal
A1	2	1/2
A2	4	1/4
A3	1	1

Multiply the reciprocal numbers by 4

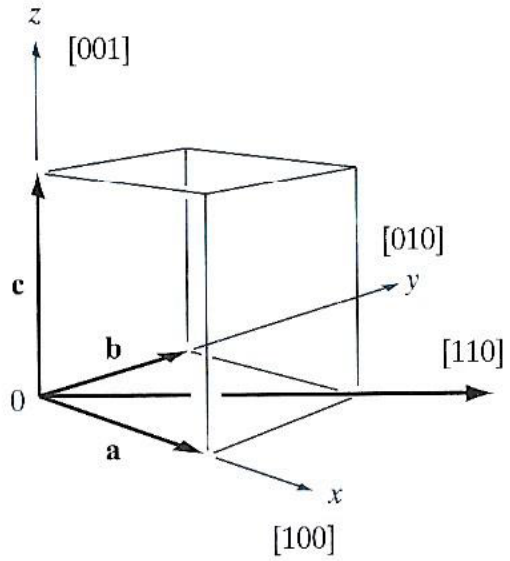
→ **Miller indices (214)**

Miller index of direction

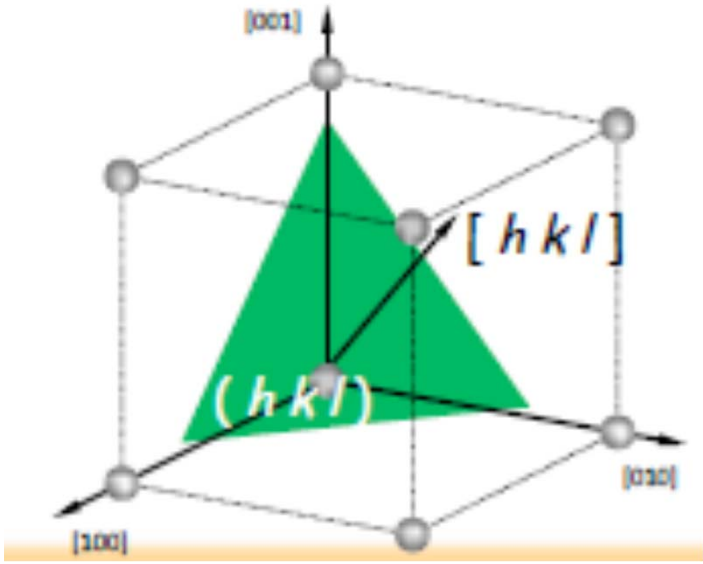
- Direction: is expressed as a set of 3 integers with same relationship as the components of a vector in that direction.



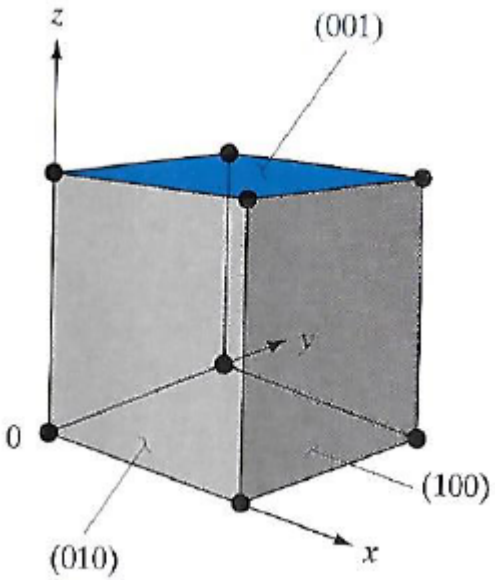
(a)

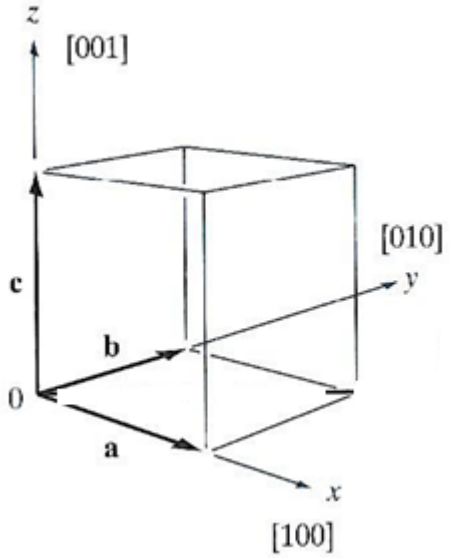


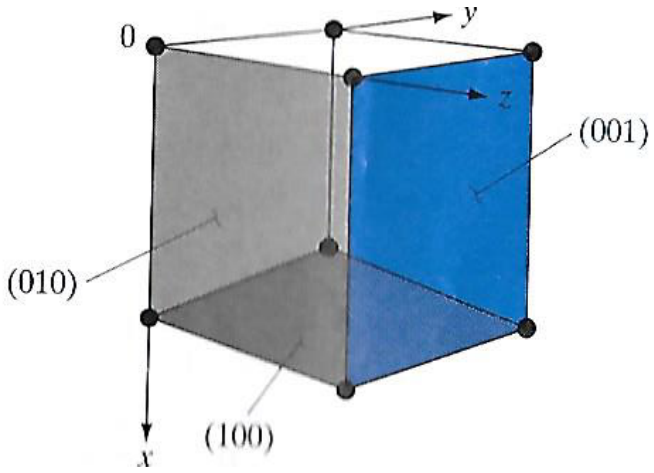
(b)



- Equivalent planes and directions:

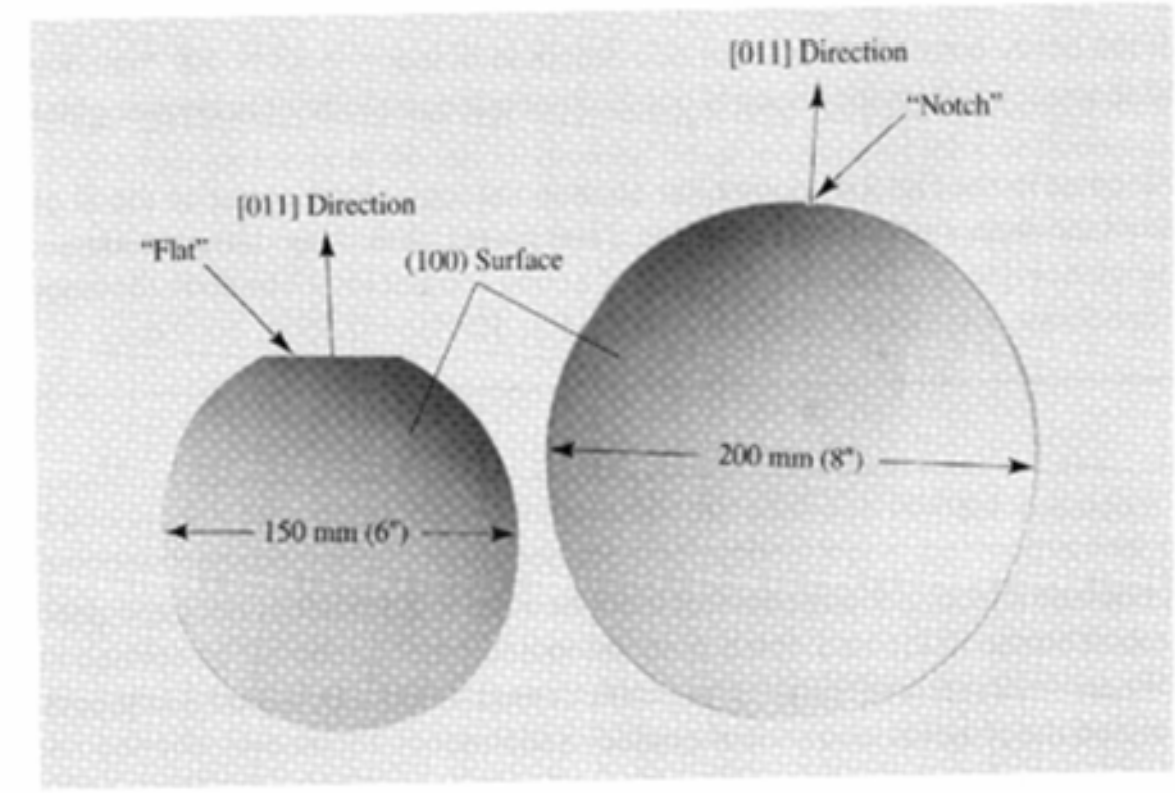






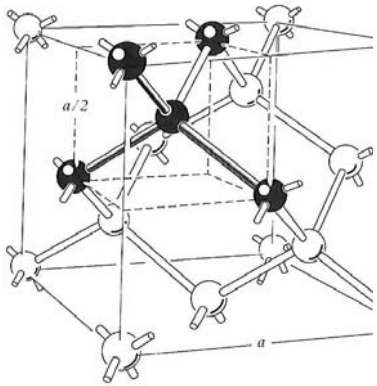
Notation	Interpretation
(*h k l*)	crystal plane
{ *h k l* }	equivalent planes
[*h k l*]	crystal direction
< *h k l* >	equivalent directions

- Si wafers usually cut along {100} plane with a notch or flat side to orient the wafer during fabrication



Key points in chapter 1 Crystal properties

1. The conductivity of semiconductor is in between insulator and metal.
2. Primitive cell is the smallest unit cell, only has lattice point at the corners; unit cell allows lattice points not only at the corners, but also at the face or body centers.
3. Three type of cubic lattice structure: simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc)
4. Crystal plane and directions are denoted by Miller indices (hkl) and [hkl]; Equivalent planes and directions are denoted by {hkl} and <hkl>.
5. Diamond structure and zinc blende structure: fcc lattice with an extra atom places at **a**/4+**b**/4+**c**/4 from each of the fcc atoms.
   If the atoms are all similar: diamond structure.
   If the atoms differ on alternating sites: Zinc blende structure.



Basic units

$$1mm=10^{-3}\ m$$

$$1\mu m=10^{-6}\ m$$

$$1nm=10^{-9}\ m$$

$$1Å=10^{-10}\ m$$

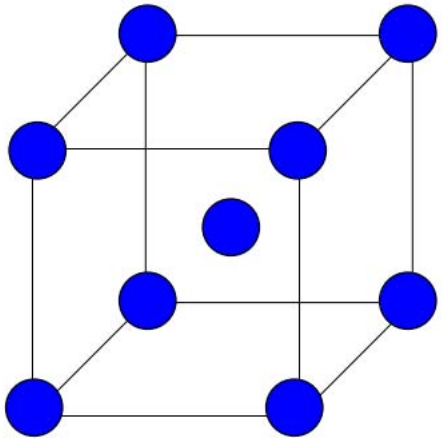
Elementary charge (e or q): 1.602×10^{-19} C

Electron volt (eV) is the amount of energy gained (or lost) by the charge of a single electron moved across an electric potential difference of one volt.

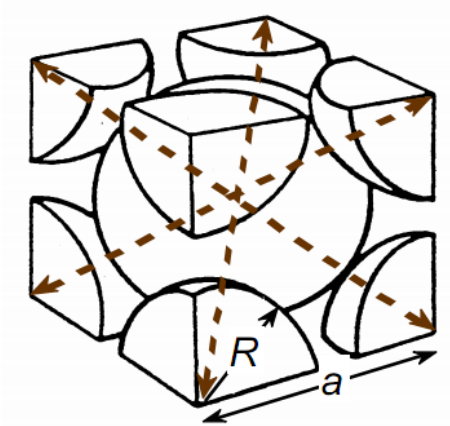
$$1eV=1.6x10^{-19}C*V=1.6x10^{-19}J$$

Example 1

What is the atomic density of a BCC material with lattice constant 5.2 angstroms?



Example 2



- Ex: Cr (BCC)

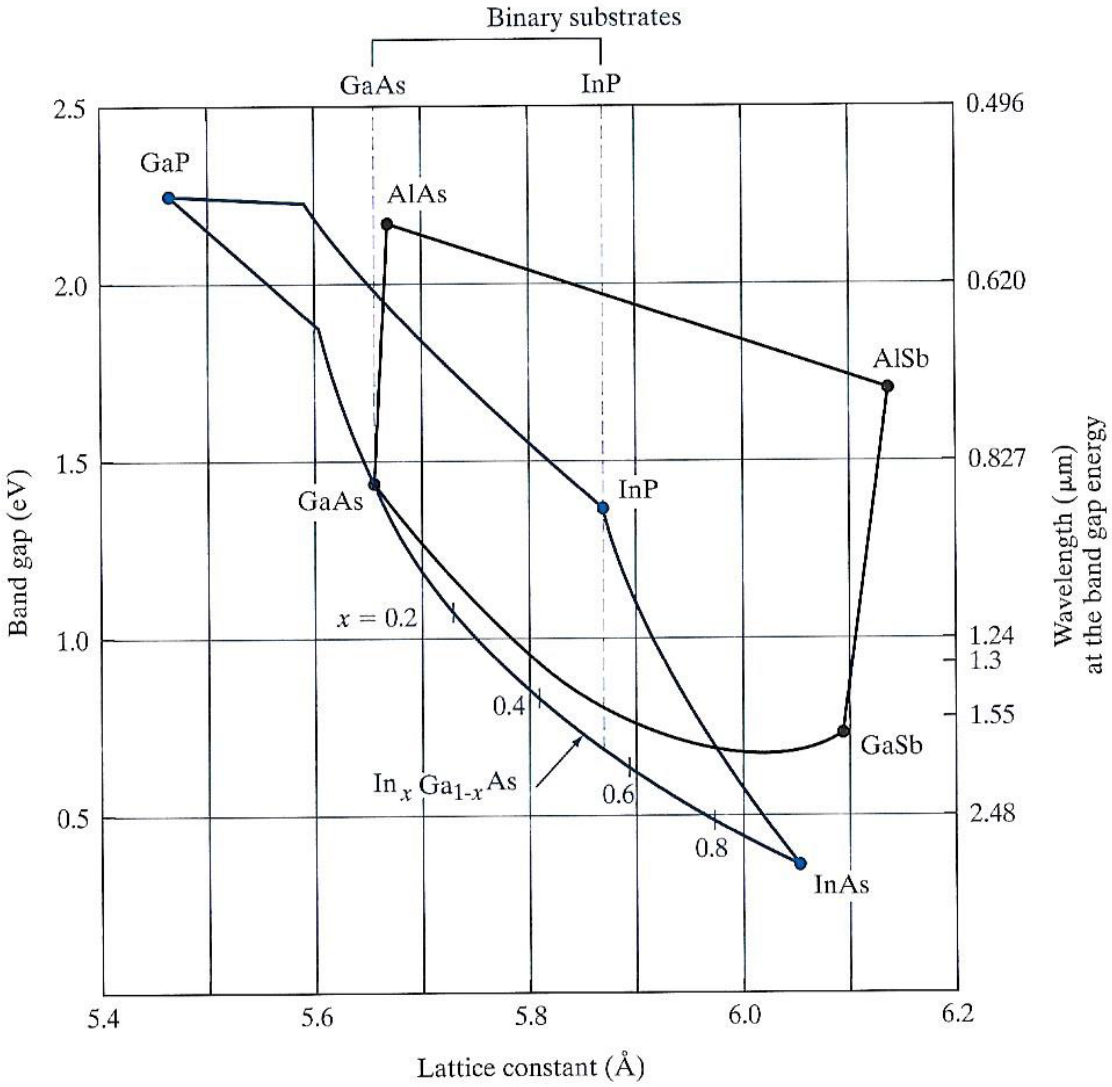
$A = 52.00$ g/mol

$R = 0.125$ nm

Avogadro's number
(6.023×10^{23} atoms/mol)

What is the mass density?

Band gap and lattice constant



$In_xGa_{1-x}As$