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EE-606: Solid State Devices
Lecture 2: Geometry of Periodic Crystals

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Outline

1) **Volume & surface issues for BCC, FCC, Cubic lattices**
2) Important material systems
3) Miller indices
4) Conclusions

Reference: Vol. 6, Ch. 1 (pages 10-17)

Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

The story so far …

1. We want to compute current in a material, J=q n v

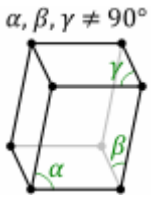
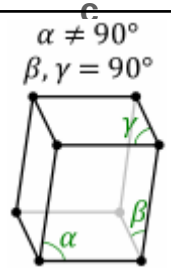
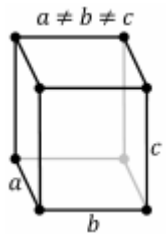
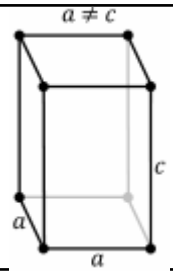
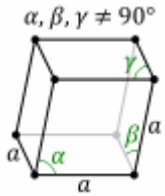
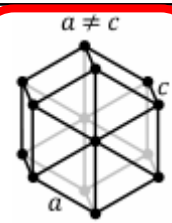
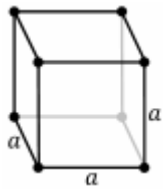
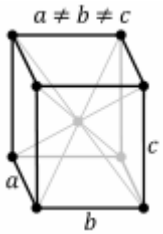
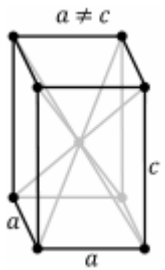
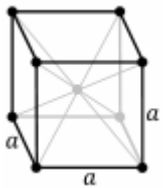
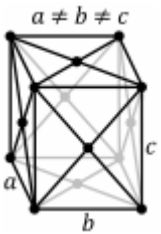
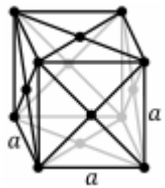
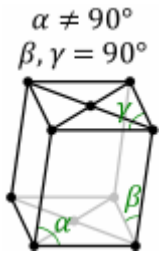
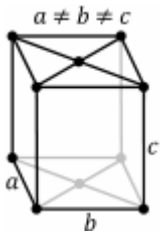
2. Computing (n) and (v) requires knowledge of composition and periodicity of the material

3. If the atoms are arranged in a periodic array, then calculation of (n) and (v) will be easier.

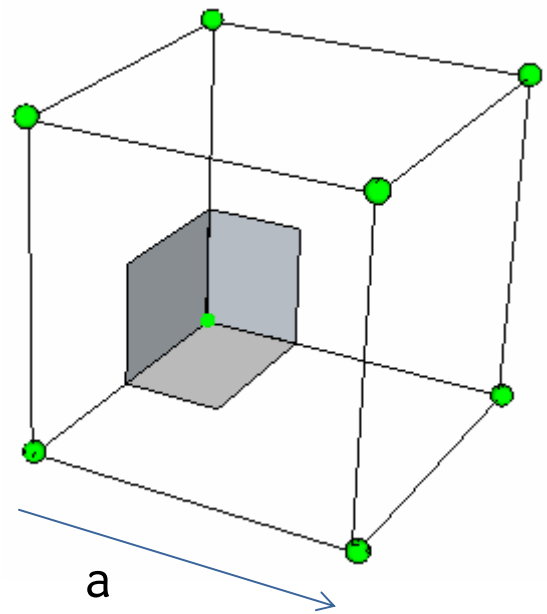
Therefore, we are studying the symmetry of the unit cell, hoping that we will be able to identify them in various materials.

Important Bravais lattices

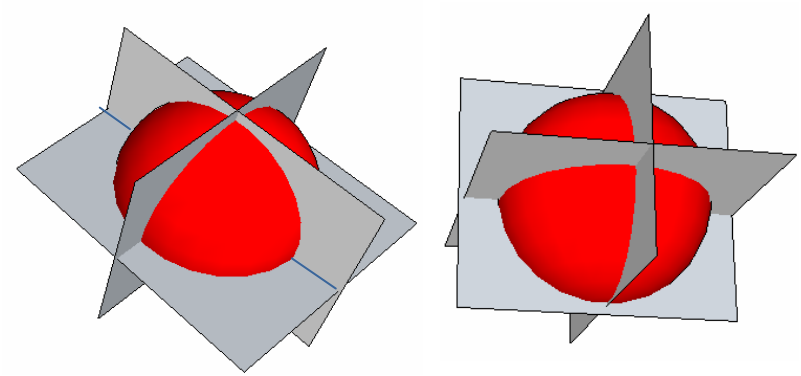
Polonium84

	Triclinic	Monoclinic	Orthorhombic	Tetragonal	Rhombohedral	Hexagonal	Cubic
P							
I							
F							
C							

Cubic Lattice: Volume Issues

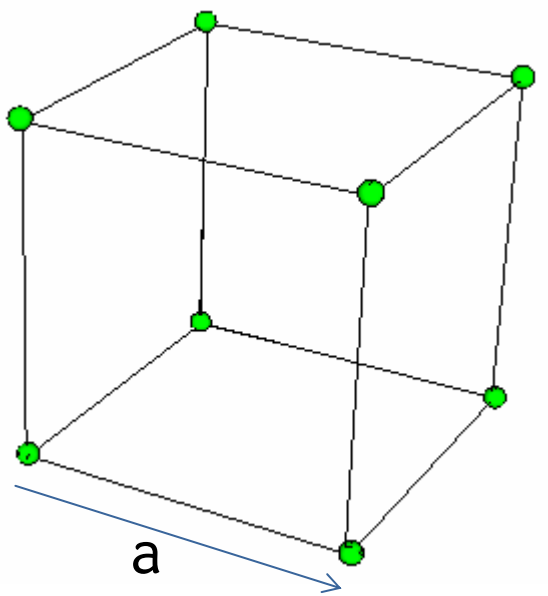


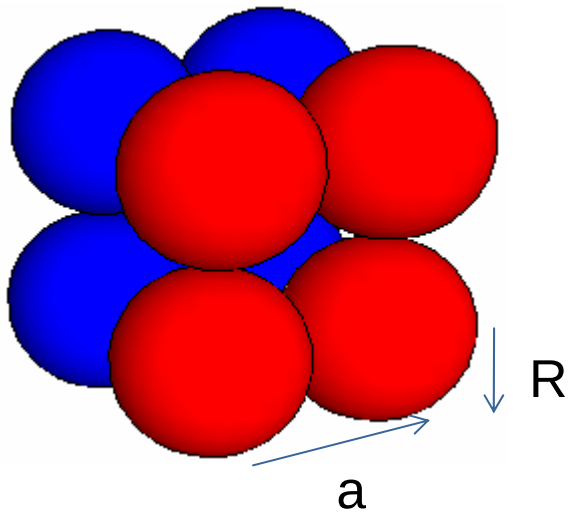
Points per cell
=1/8 points/corner x 8 corners
=1 Point/cell.
(depends on definition of cell)



Number density
= $(1/a^3)$ points/cm^3.
(does not depend on cell definition)

Cubic Lattice: Volume Issues





Packing density
=volume filled/total volume

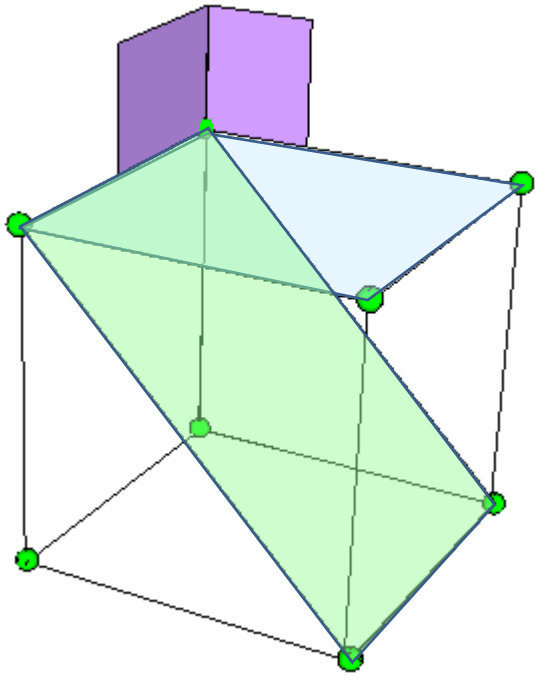
R=a/2

P= (1/8)x(4/3)πR^3 x (8 corners) /a^3

$=\pi/6$

(does not depend on cell definition)

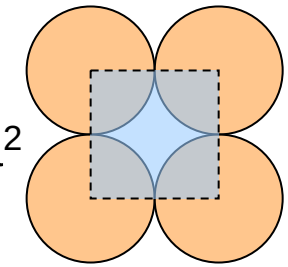
Cubic Lattice: Surface Issues

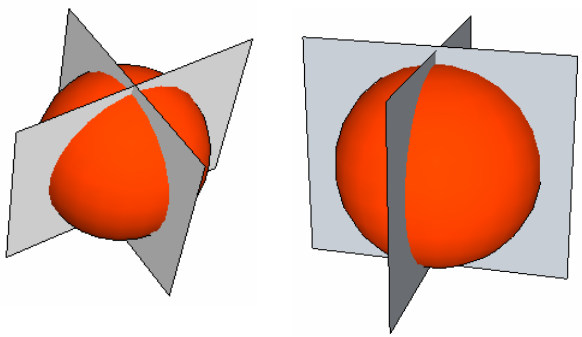


Areal Density

=(1/4 per corner) x (4 corners)/a^2

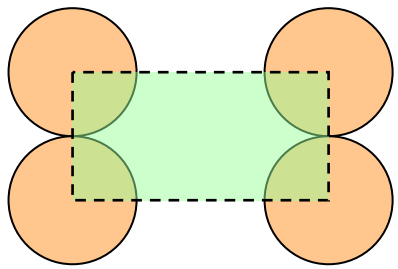
=$1/a^2$ cm^{-2}



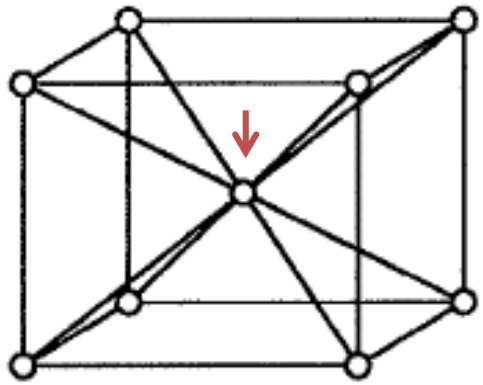


Areal density (face diagonal)

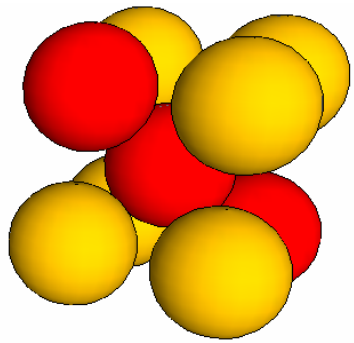
= (1/4 points/corner) x (4 corners)/$\sqrt{2}a^2$ cm^{-3}

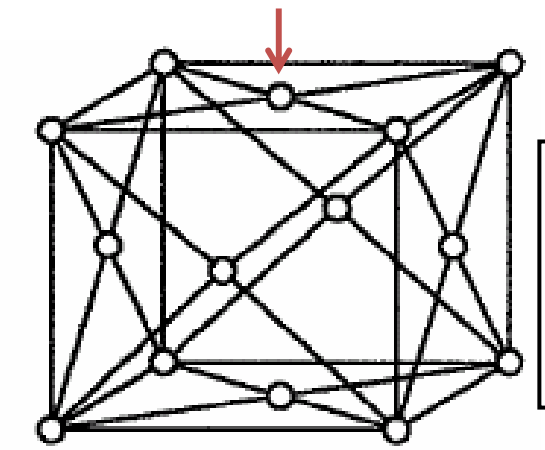


BCC and FCC lattices

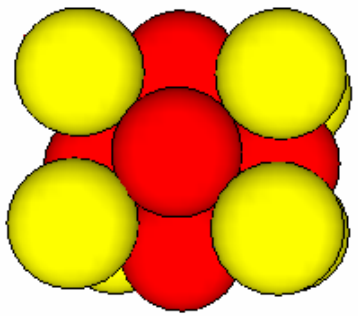


Points per cell
= 1/8 x 8 @corners
+ 1 @inside
=2

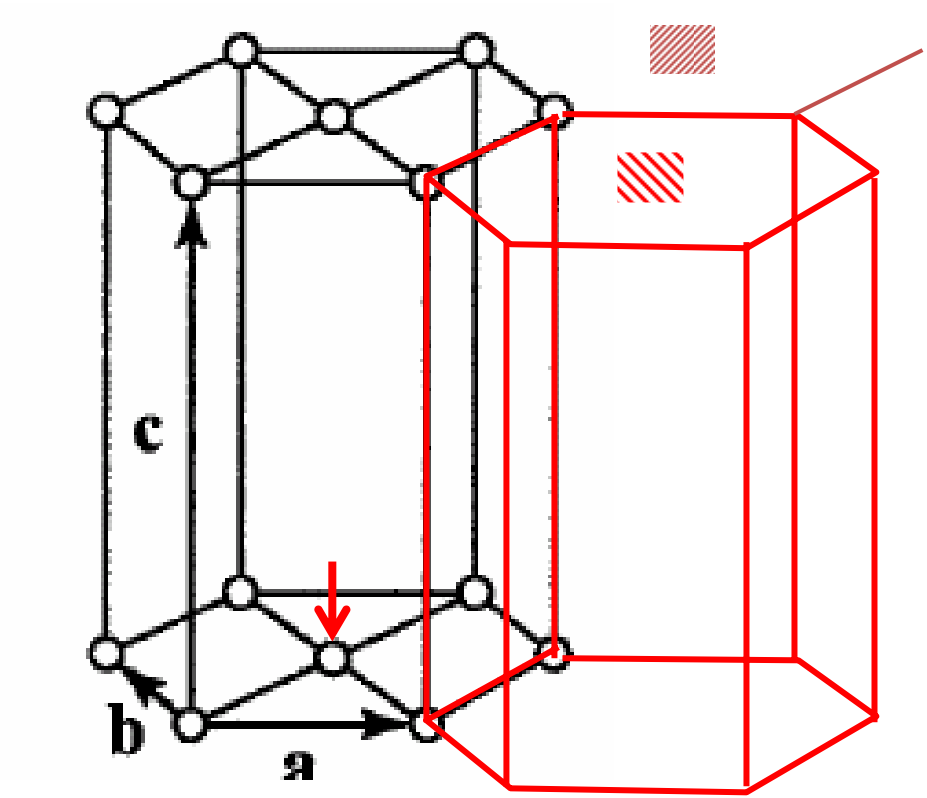




Points per cell
= 1/8 x 8 @corners
+ 1/2 x 6 @faces
=4

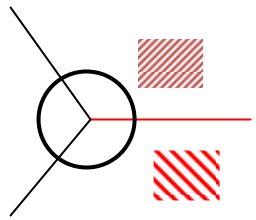


Hexagonal Closed-Packed



Points per cell

1/2 x 2 @faces =1



1/2x1/3 x 12 @corners =2

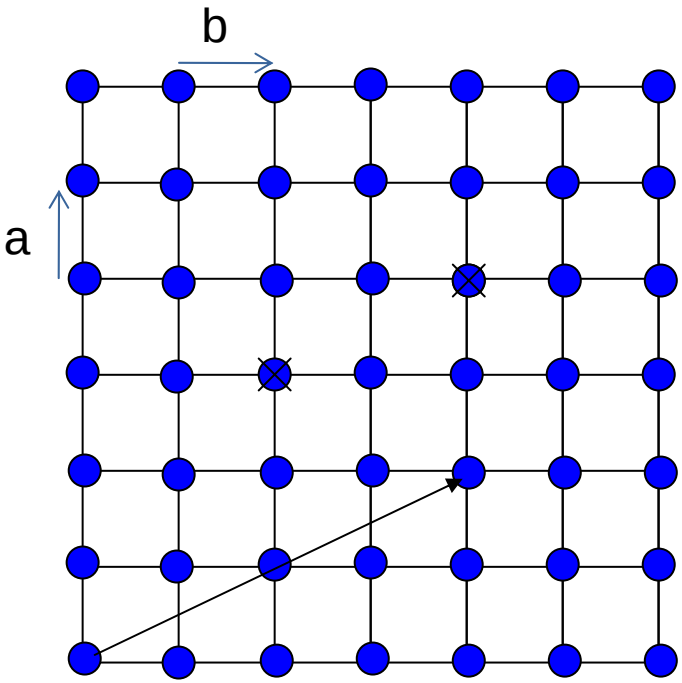
3 points/cell

Outline

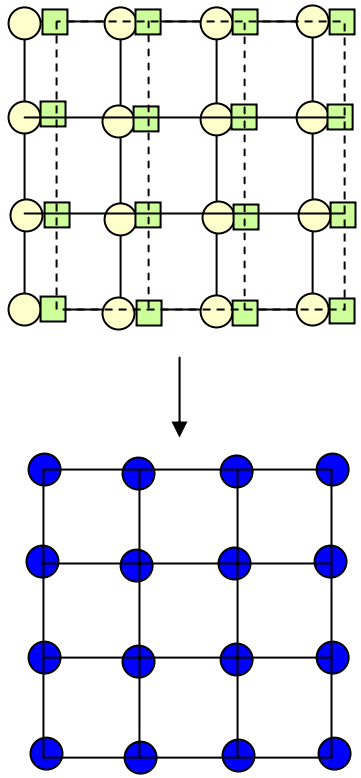
1) Volume & surface issues for BCC, FCC, Cubic lattices
2) **Important material systems**
3) Miller indices
4) Conclusions

Geometry of Lattice Points

In a Bravais lattice, every point has the same environment as every other point (same number of neighbors, next neighbors, …)



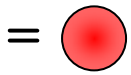
$$R = h\vec{a} + k\vec{b}$$

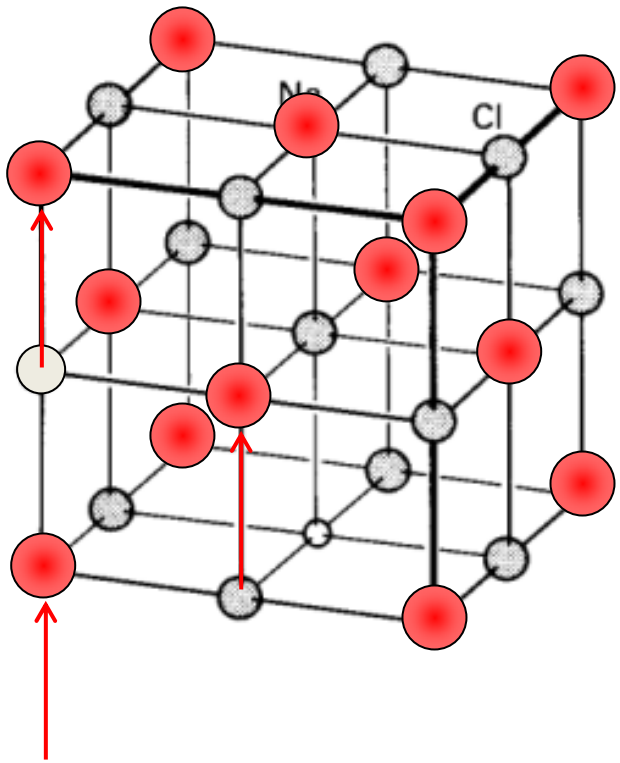


Non-Bravais lattice

Bravais lattice with a basis

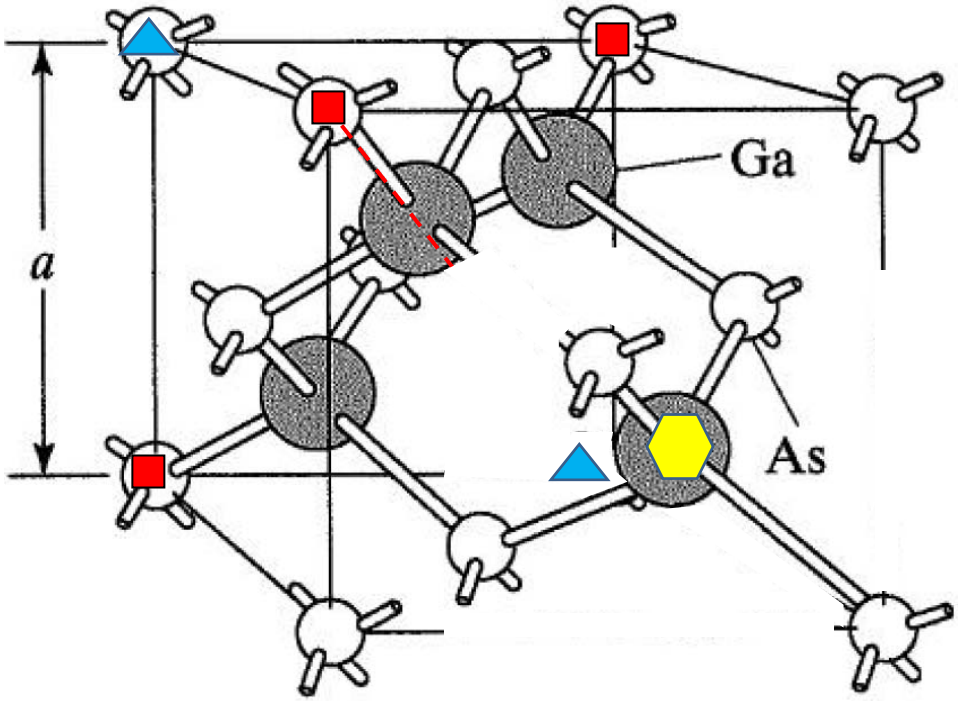
Rock-Salt as FCC lattice

= 

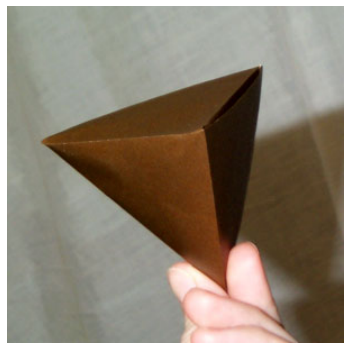


For more discussion, see Kittle and Ashcroft/Mermin

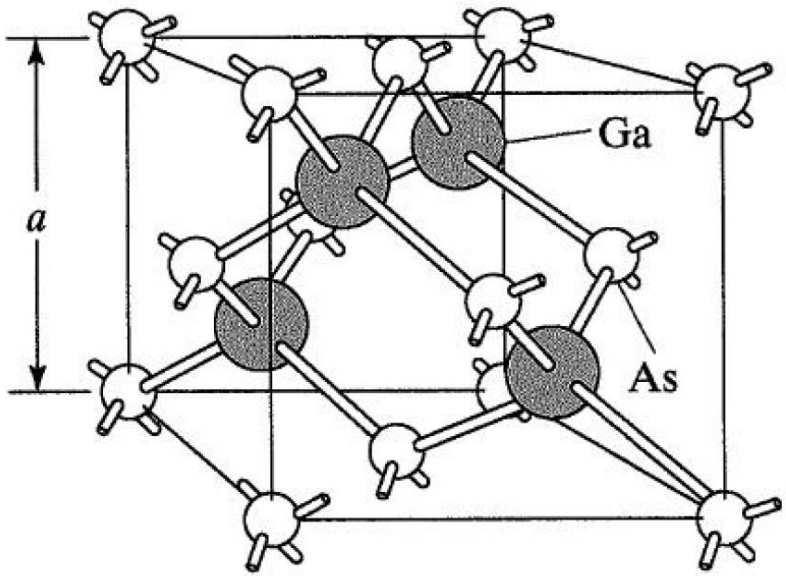
Zinc-Blende FCC Lattice for GaAs

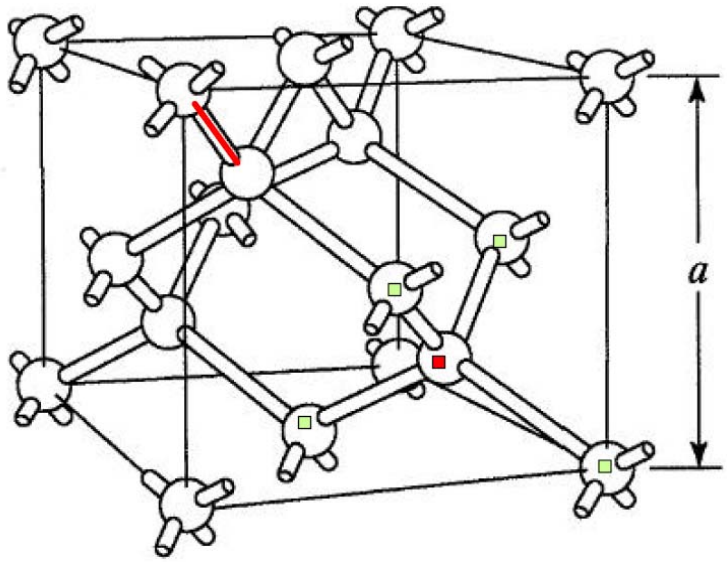


Atoms/cell=(1/8)x8 + (1/2)x6 + 4=8
FCC Lattice with a basis
Tetrahedral structure

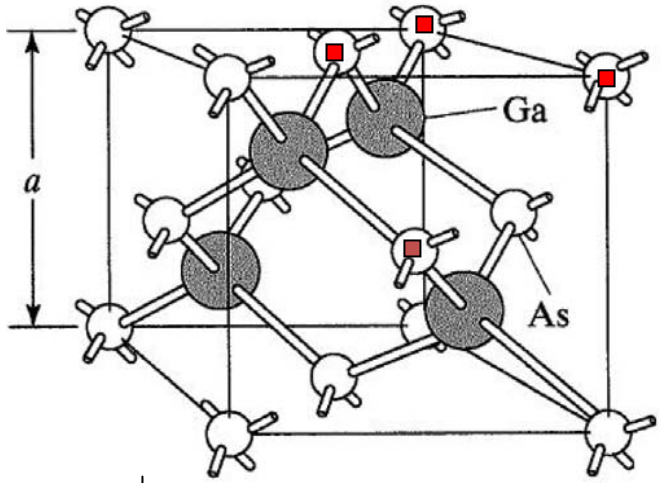


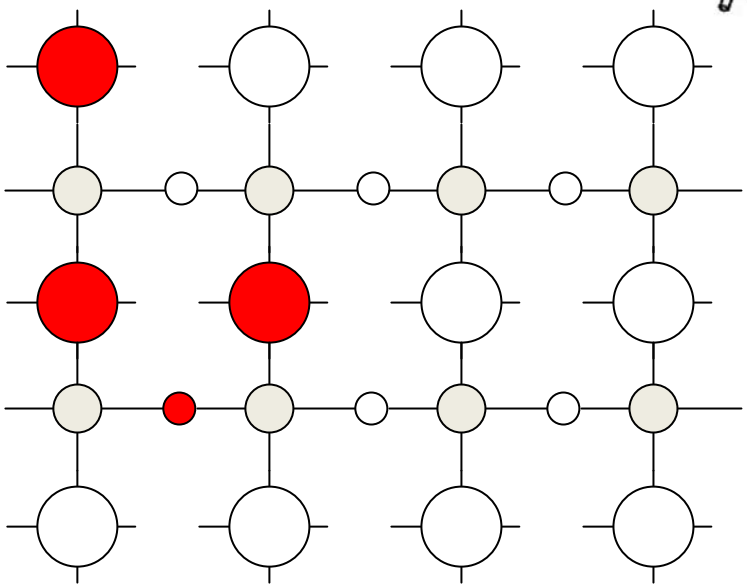
Diamond FCC Lattice for Silicon

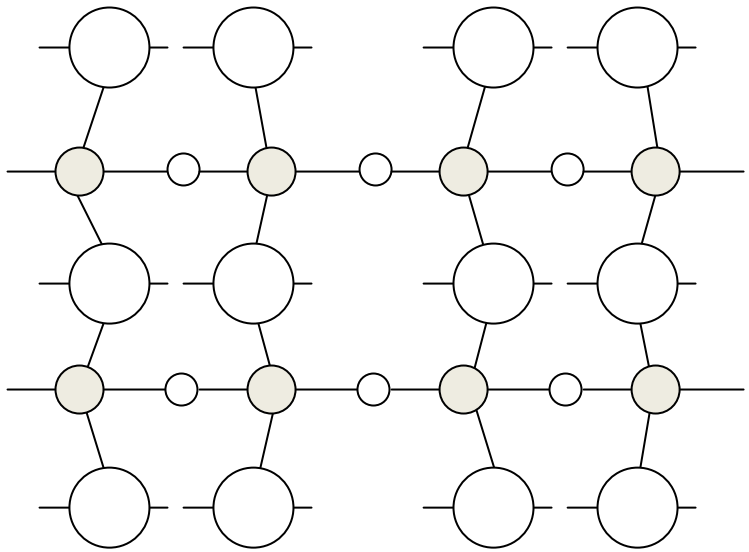




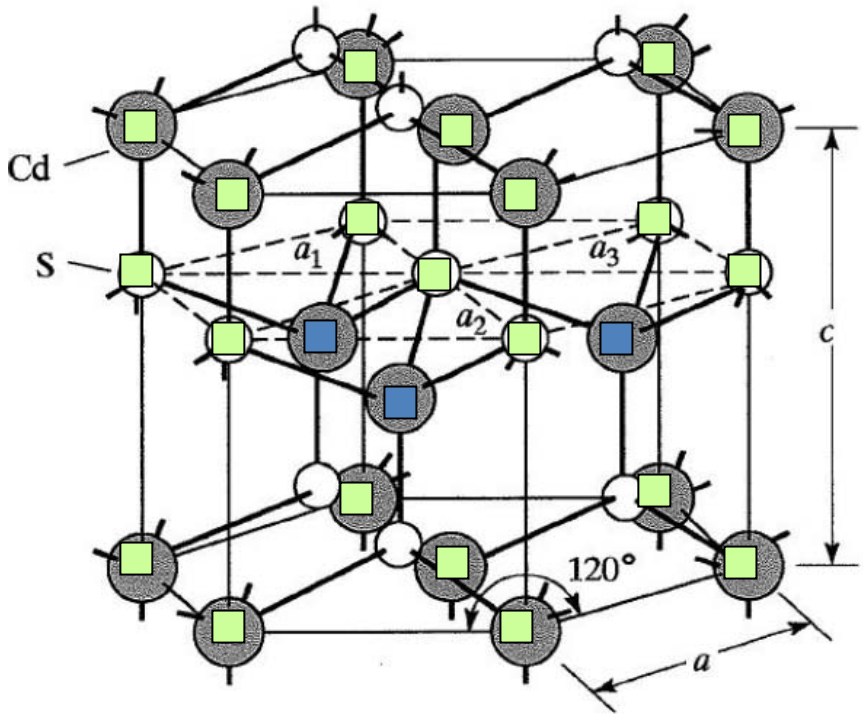
Surface Reconstruction



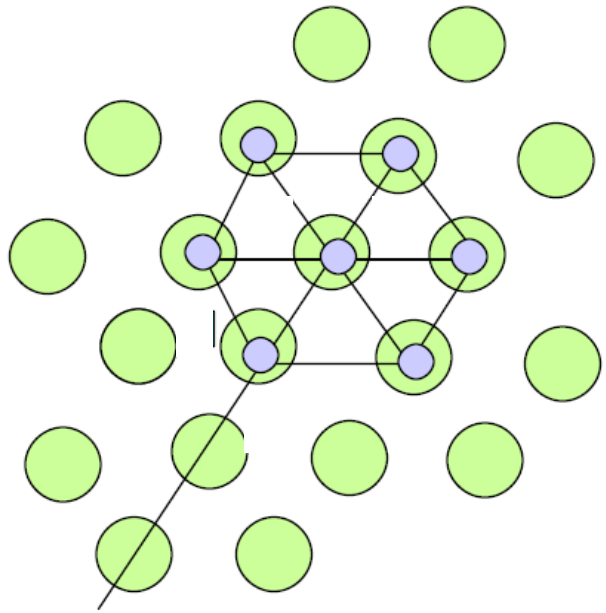




Hexagonal Closed-Packed for CdS



Focus on (Cd) …

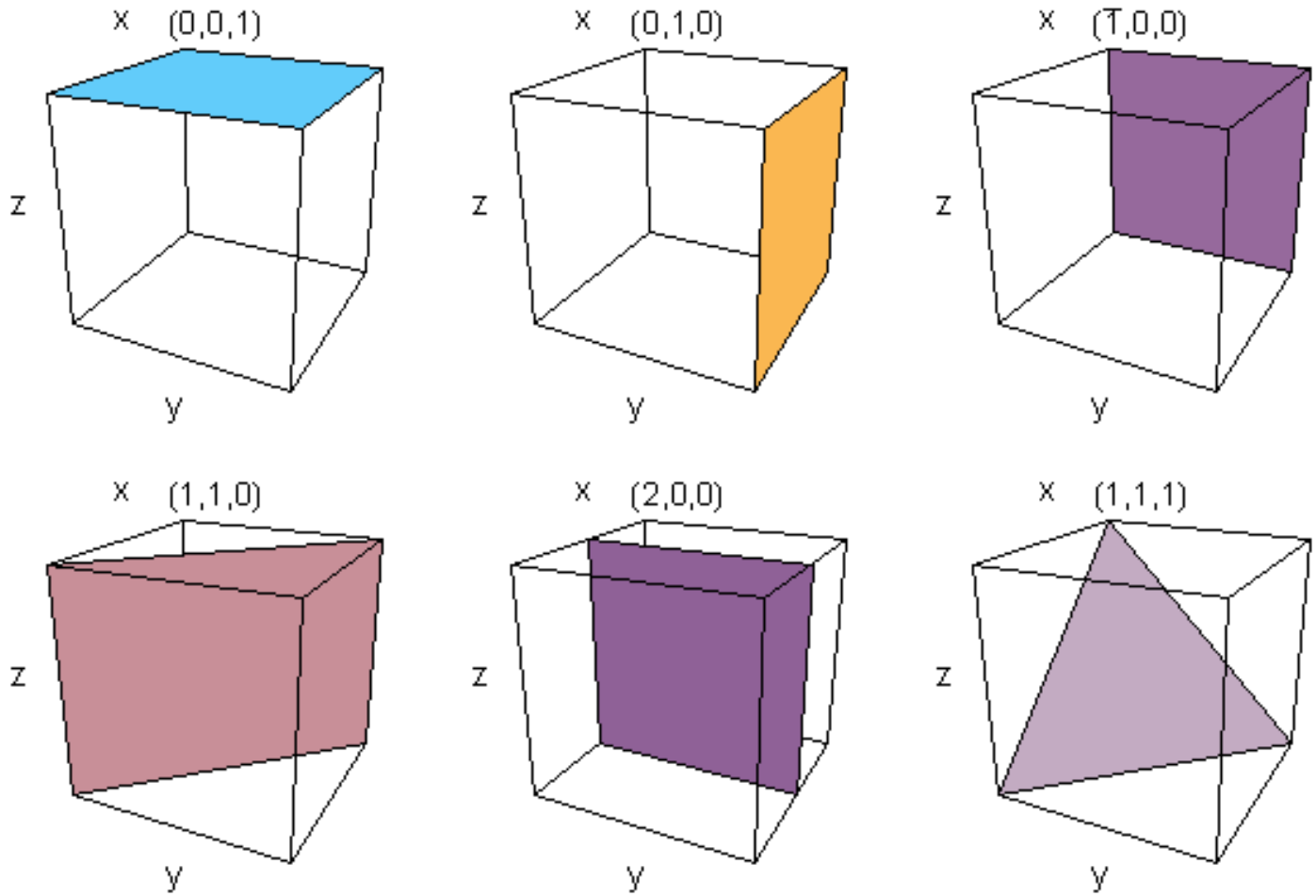


(Cd) atoms/cell=
(1/6)x12 + (1/2)x2 + 3=6

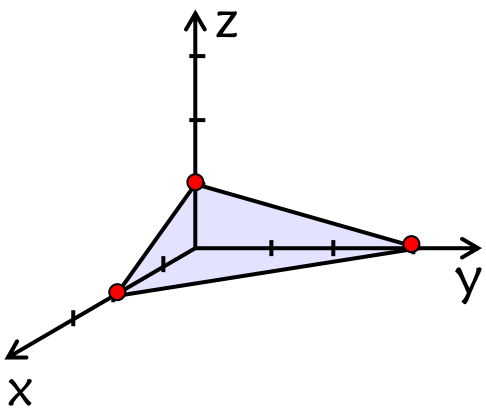
Outline

1) Volume & surface issues for BCC, FCC, Cubic lattices
2) Important material systems
3) **Miller indices**
4) Conclusions

Miller-Indices and Definition of Planes



Miller Indices: Rules



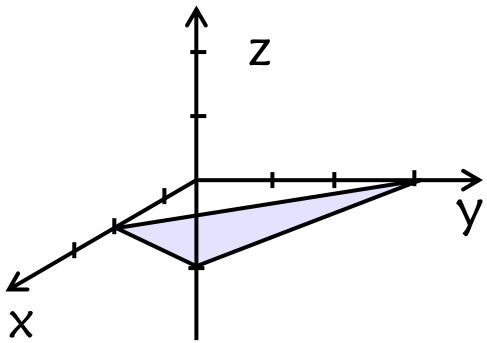
1. Set up axes along the edges of unit cell
2. Normalize intercepts …. 2, 3, 1
3. Invert/rationalize intercepts … 1/2, 1/3, 1

   3/6, 2/6, 6/6
4. Enclose the numbers in curvilinear brackets

   (326)

Few more rules …

Negative Intercept



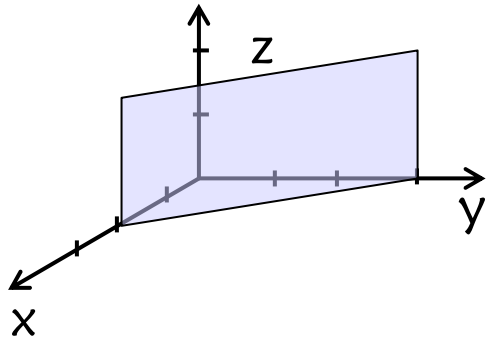
2, 3, -2

1/2, 1/3, -1/2

3, 2, -3

(3 2 $\bar{3}$)

Intercept at infinity



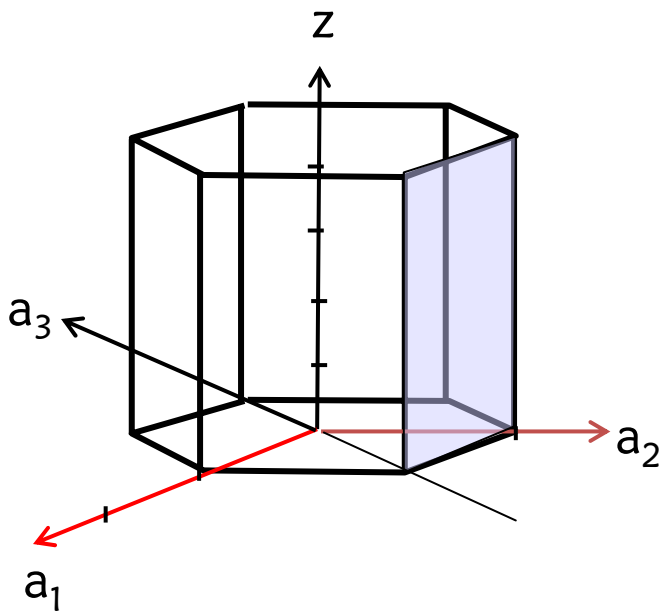
2, 3, ∞

1/2, 1/3, 0

3, 2, 0

(3 2 0)

Bravais-Miller Indices



∞, 1, -1, ∞

0, 1, -1, 0

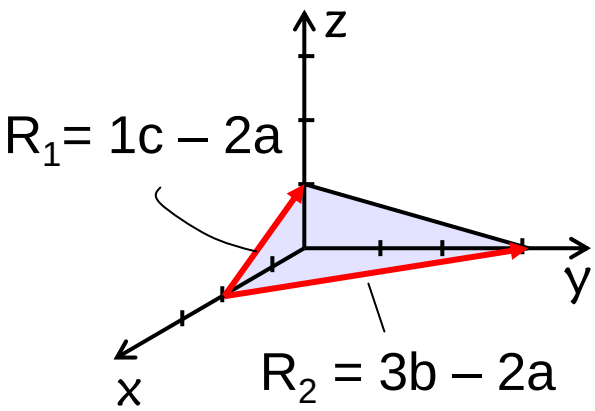
0, 1, -1, 0

$(0\ 1\ \bar{1}\ 0)$

First three indices sum to zero.

Where does Miller Indices come from ?

Miller indices: (326)



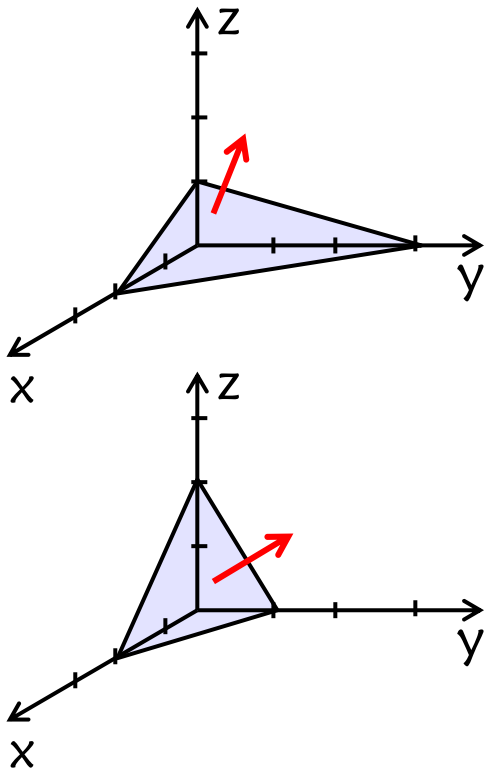
Normal to the surface

$$R_2 x R_1 = \begin{vmatrix} a & b & c \\ -2 & 3 & 0 \\ -2 & 0 & 1 \end{vmatrix} = 3a + 2b + 6c$$

Vector indices same as Miller indices !

(326) vs. [326]

Angle between Two Planes



Unit vector normal to plane 1:

$$N_1 = (h_1\vec{a} + k_1\vec{b} + l_1\vec{c})/(h_1^2 + k_1^2 + l_1^2)^{1/2}$$

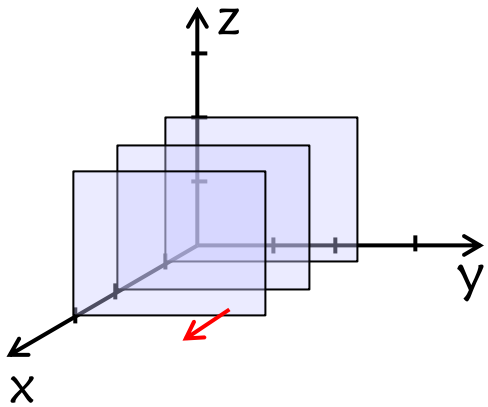
Unit vector normal to plane 2:

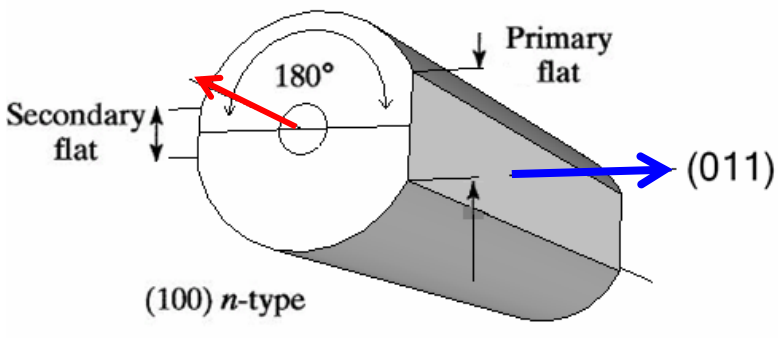
$$N_2 = (h_2\vec{a} + k_2\vec{b} + l_2\vec{c})/(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

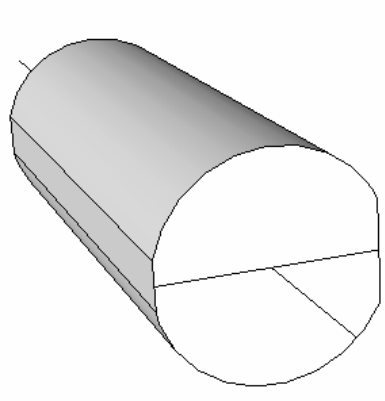
$$Cos(\theta) = N_1 \bullet N_2$$

$$= (h_2h_1 + k_2k_1 + l_2l_1)/(h_2^2 + k_2^2 + l_2^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

Examples …





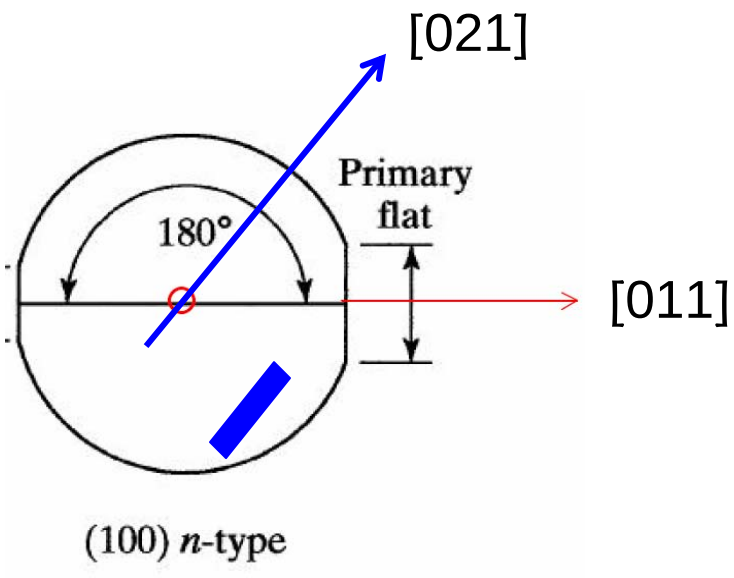


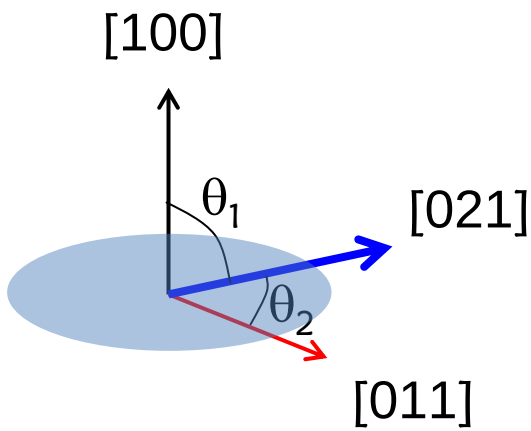
$\cos(\theta)=(1x0+0x1+0x1)/(\sqrt{1}x\sqrt{2}) = 0$

so θ=90 degrees

(011) surface is normal to (100) surface

Example use of Miller Indices .. Find [021] Direction





$\cos(\theta_1)=(1x0+0x2+0x1)/(1x\sqrt{5}) = 0$, so $\theta_1=90$ degrees

[021] vector lies on (100) plane.

$\cos(\theta_2)=(0x0+2x1+1x1)/(\sqrt{5}\ \sqrt{2})$, so $\theta_2=18.5$ degrees with respect to [011] direction.

Conclusions

1. To understand transport in semiconductors, we need to know carrier density (n) and carrier velocity (v). In order to find these quantities, we need to understand the chemical composition and atomic arrangements.

2. Crystalline material can be built by repeating the basic building blocks. This simplifies the quantum solution of the material, which will allow us to compute n and v for these systems easily.

3. Silicon, GaAs, PbS do not have simple Bravais lattice; but they have Bravais lattice with basis.

4. Often we need to calculate the direction of crystal planes because material properties differ along different planes. Miller indices are one useful way of characterizing crystal planes. In is useful to to review some identities of vector calculus to such calculations involving crystal planes.

Looking ahead ….

Number of atoms/volume
from crystal structure

Number of electrons
available for conduction

Number of electrons/atoms

$$n \neq \rho \times N$$

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 **Al**	14 **Si**	15 **P**	16 S
30 **Zn**	31 **Ga**	32 Ge	33 **As**	34 **Se**
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

All electrons may be created equally,
but they appear do not behave identically!