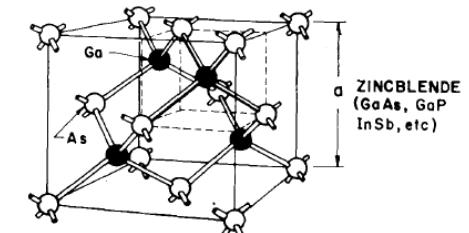
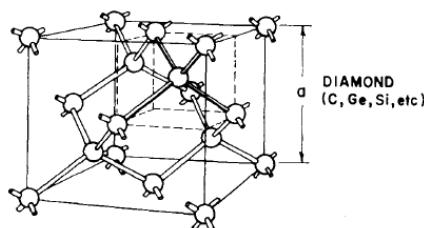


# 618327-2560

## PHYSICS OF ELECTRONIC MATERIALS AND DEVICES

Dr. Orrathai Watcharakitchakorn

### Lecture 1



# Basic Crystal Structure

โครงสร้างผลึก

ຂອງແຈ້ງແບ່ງປັນ 3 ອິຫາຍ່ອຍ

1. Solids may be classified into **3** groups:

>> Amorphous

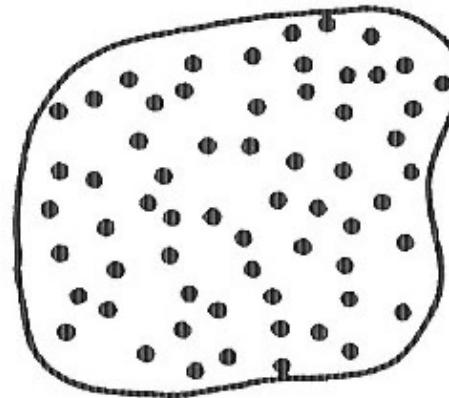
>> Polycrystalline

>> Crystalline

# Basic Crystal Structure

- 1.1. **Amorphous:** Atoms are randomly arranged (formlessness).

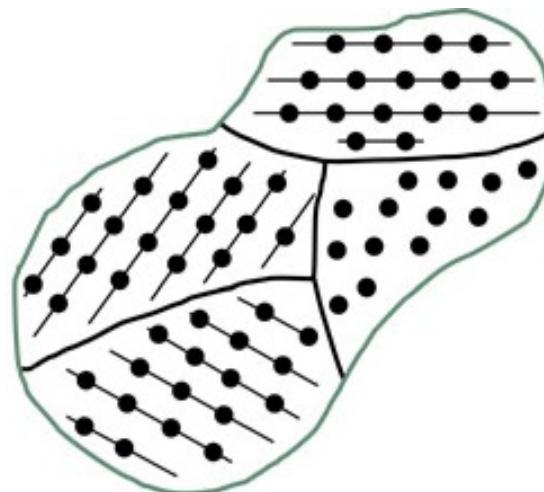
ของแข็งประเภทนี้ไม่เป็นรูปทรงตัวใดๆ เช่น แก้ว ยาง พลาสติก



# Basic Crystal Structure

- 1.2. • **Polycrystalline:** Atoms have many small regions. Each region has a well organized structure but differs from its neighboring regions.

ของแข็งประเภทนี้ไม่เลกุลของมันจะเรียกตัวเป็นระเบียบที่แน่นอนอย่างหนึ่ง  
รวมกันขึ้นเป็นผลึก(Crystal) เช่น ผลึกของเกลือแร่ NaCl เพชร

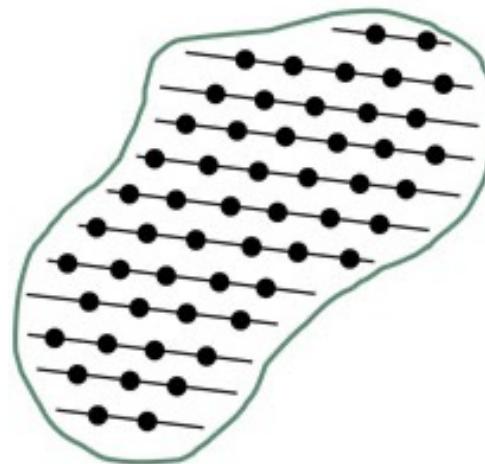


# Basic Crystal Structure

- 1.3. • **Crystalline:** Atoms are arranged in an orderly array.

ของแข็งที่หน่วยโครงสร้างมีตัวແண່ງ ที่แน่นอนและเรียบตัวเป็นระเบียบ

ຈຳສາງອັນໄລວິນນີ້ຕົວເລີ່ມຈາກ



# Basic Crystal Structure

คำ  ภาษาอังกฤษ

- **Crystal** (ผลึก) : มองจากภายนอกผลึกจะมีรูปทรงที่แน่นอน มีผิวเรียบ เมื่อ grow จะไม่เปลี่ยนรูปถ้ามองลึกเข้าไปถึงระดับอะตอม ผลึกจะประกอบด้วยอะตอมหรือกลุ่มของอะตอมที่จัดตัวอย่างเป็นระเบียบและมีลักษณะซ้ำกัน (periodic array of atom)

ในการเขียนโครงสร้างของผลึกมักจะใช้จุดแทนตำแหน่งของอะตอมหรือแทนตำแหน่งของกลุ่มอะตอมที่มีลักษณะซ้ำๆ กันนั้นจุดนี้เรียกว่า Lattice point หรือ lattice และอะตอมหรือกลุ่มอะตอมซึ่งแทนด้วย lattice เรียกว่า basis

↑  
ภาษาอังกฤษ: atom

# Basic Crystal Structure

- A collection of point periodically arranged is called a **lattice**. จุดแทนตำแหน่งของอะตอมหรือแทนตำแหน่งของกลุ่มอะตอมที่มีลักษณะซ้ำ ๆ กันนั้น
- Lattice contains a volume called a **unit cell** which is representative of the entire lattice. คือหน่วยที่เล็กที่สุด ที่แสดงลักษณะการเรียงตัวของหน่วย โครงสร้างอย่างสมบูรณ์
- By repeating the unit cell throughout the crystal, one can generate the entire lattice.

# Unit cell

- Unit cell has an atom at each corner shared with adjacent cells.
- This unit cell is characterized by integral multiples of vectors such as  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  called **basis vectors**.
- Basis vectors are not normal to each other and not necessarily equal in length.

Basis Vector : គីអ៊ីតុសទូទៅនៃការបង្កើតការងារ

$m\mathbf{a}$ ,  $n\mathbf{b}$ ,  $p\mathbf{c}$  ;  $m, n, p$  គឺជាតាមលេខ 1, 2, 3, ...  
 $a, b, c$  គឺជាបឋមវិបីតុស

# Unit cell

Every equivalent lattice point in the crystal can be expressed by

- Two-dimensional case:  $\text{ฉบับ } m,n ; x,y$

$$\mathbf{r} = m\mathbf{a} + n\mathbf{b} \quad \mathbf{a}, \mathbf{b} : \text{basic vector}$$

- Three-dimensional case:  $\text{ฉบับ } m,n,p ; x,y,z$

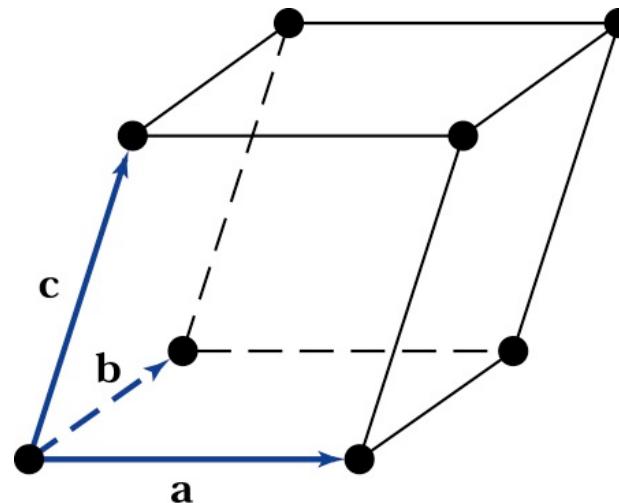
$$\mathbf{r} = m\mathbf{a} + n\mathbf{b} + p\mathbf{c} \quad \mathbf{a}, \mathbf{b}, \mathbf{c} : \text{basic vector}$$

where  $m, n$ , and  $p$  are integers

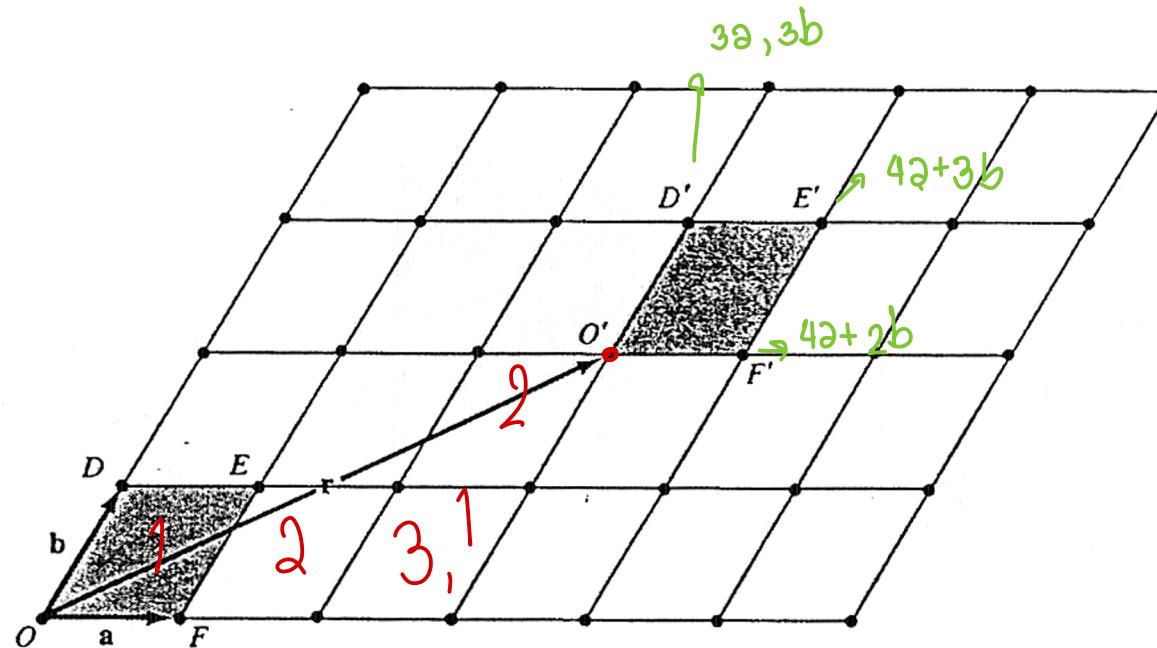
# Unit cell

- The smallest unit cell that can be repeated to form the lattice is called a **primitive cell** shown below.

խնդիր 1



# Unit cell



Ex. 2-D lattice

$$\mathbf{r} = 3\mathbf{a} + 2\mathbf{b}$$

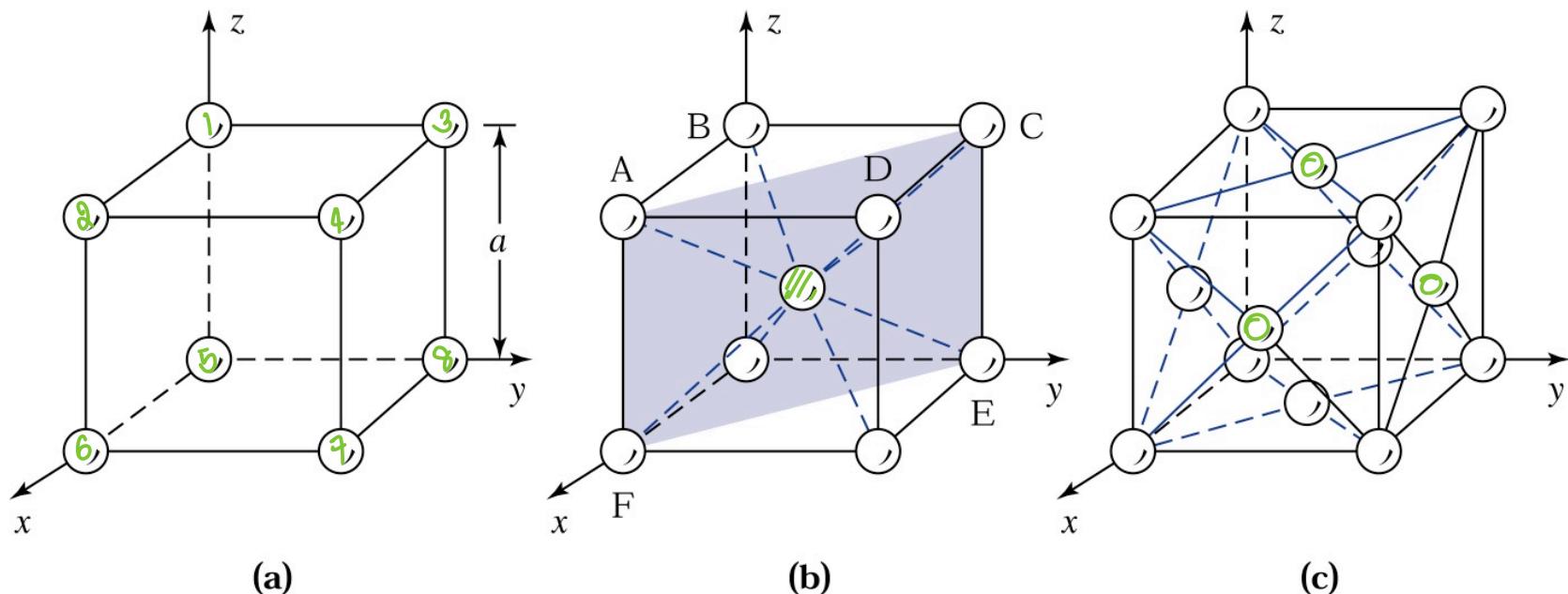
↓  
380)

# Basic Crystal Structure

โครงสร้างผลึก

มี 3 ตัวอย่างดังนี้

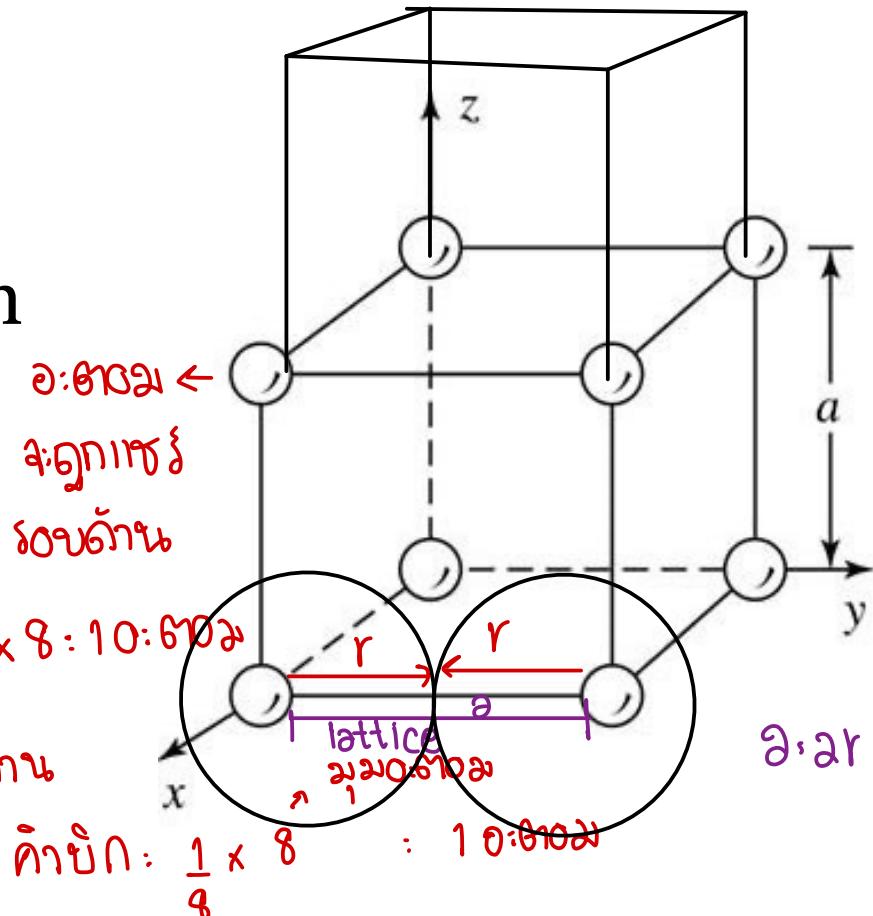
- There are three basic cubic-crystal structures:
  - (a) simple cubic (โครงสร้างคิบิกซึ่งมีองศาเรียบ)
  - (b) body-centered cubic (โครงสร้างคิบิกศูนย์กลางในตัว)
  - (c) face-centered cubic (โครงสร้างคิบิกหน้าร่อง)



# Simple cubic

- Each corner of cubic lattice is occupied by an atom which is shared equally by *eight* adjacent unit cells.
- The total number of atoms is equal to

$$8 \times \frac{1}{8} = 1 \text{ atom/unit cell}$$



# Simple cubic

ធនធានសំគាល់ដែលមានរាយការទៅវាង

- For the case of maximum packing (atoms in the corners touching each other), about 52% of the SC unit cell volume is filled with hard spheres, and about 48% of the volume is empty.

Atomic packing factor(PF) =  $\frac{\text{volume of atom in unit cell}}{\text{volume of unit cell}}$  នៃការងារ Unit Cell

$$PF = \frac{1 \times \left( \frac{4}{3} \pi r^3 \right)}{a^3} = \frac{\left( \frac{4}{3} \pi r^3 \right)}{(2r)^3} = \frac{\pi}{6} = 0.52$$

: 52%. ការងារ 48%. ពេលវេលា

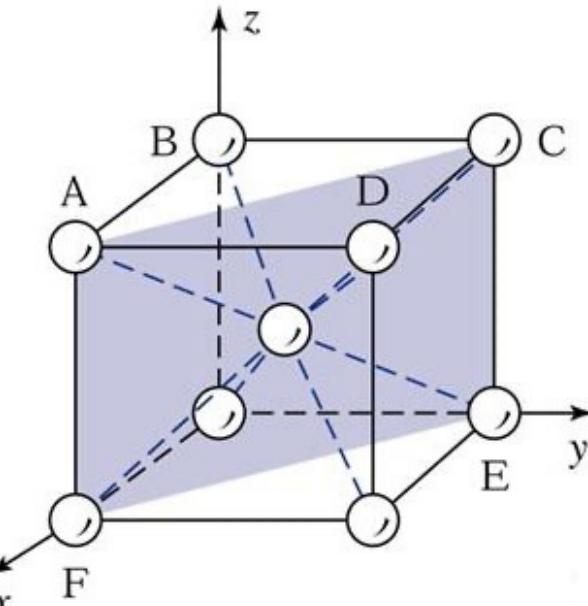
a: 2r ឬ ពេលចាប់បិតចាប់យកចាត់ 3

# Body-centered cubic (BCC)

- An additional atom is located at the center of the cube.
- The total number of atoms is equal to

$$\left(8 \times \frac{1}{8}\right) + 1 = 2 \text{ atoms/unit cell}$$

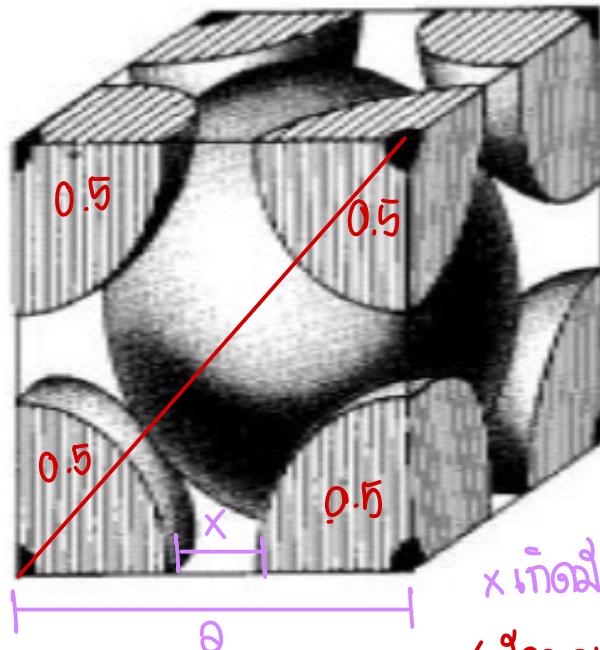
- Ex. Ba, Ce, Cr, Mo, Nb, K



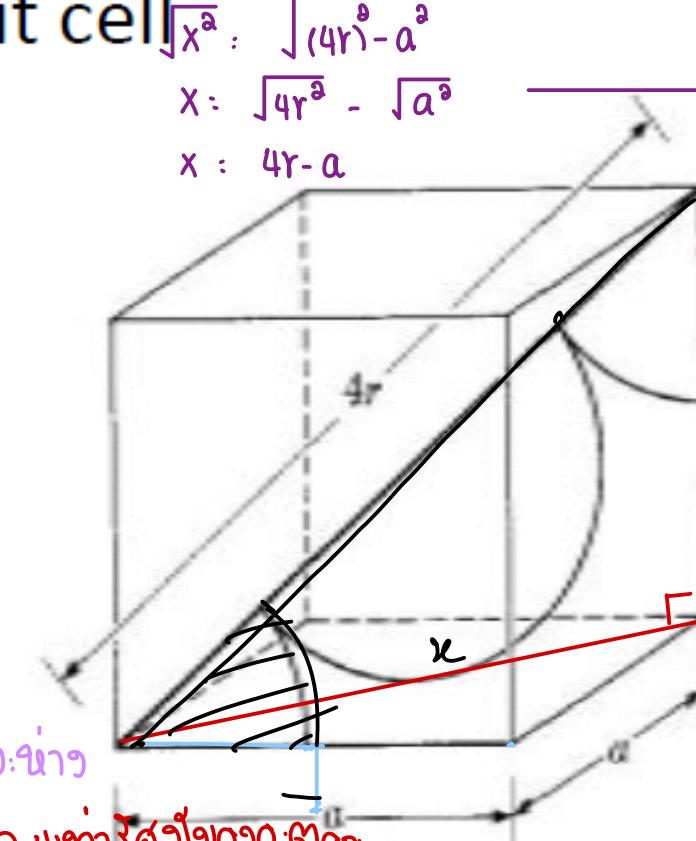
↑ ຕາງດລາງເປັນ 2 ແມ່ຕ່ລະນຸວ

$$PF = \frac{2 \times \left(\frac{4}{3} \pi r^3\right)}{a^3} = \frac{\left(\frac{8}{3} \pi r^3\right)}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

- 2 atoms in one unit cell



$x$  កែលើរៀង: ជាង  
/ តីគាមហាត 4 ការសម្រេច 090: និង



$$x^2 + a^2 = (4r)^2$$

$$x^2 = (4r)^2 - a^2$$

$$\sqrt{x^2} = \sqrt{(4r)^2 - a^2}$$

$$x = \sqrt{4r^2 - a^2}$$

$$x = 4r - a$$

$$x^2 + a^2 = (4r)^2$$

$$x^2$$

$$a^2 + a^2 = x^2$$

$$a = \frac{4R}{\sqrt{3}}$$

$$a = \frac{4R}{\sqrt{3}}$$

$$a$$

$$a^2 + a^2 = x^2$$

$$a^2 + a^2 = (4r-a)^2$$

$$2a^2 = (4r)^2 - a^2$$

$$2a^2 + a^2 = 16r^2$$

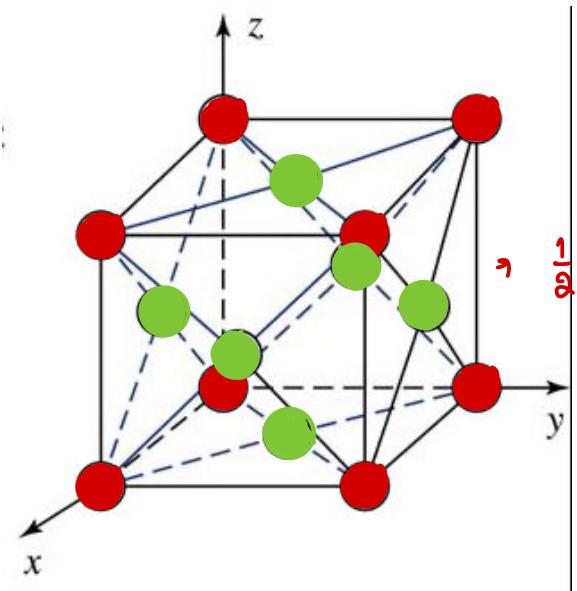
$$3a^2 = 16r^2$$

$$a^2 = \frac{16r^2}{3}$$

$$\sqrt{a^2} = \sqrt{\frac{16r^2}{3}}$$

$$\therefore a = \frac{4r}{\sqrt{3}} \# \frac{\sqrt{16r^2}}{\sqrt{3}}$$

# Face-centered cubic (FCC)



- One atom is added at each of six cubic faces in addition to the eight corner atoms.
- The total number of atoms is equal to

$$\left(8 \times \frac{1}{8}\right) + \left(6 \times \frac{1}{2}\right) = 4 \text{ atoms/unit cell}$$

$$PF = \frac{4 \times \left(\frac{4}{3} \pi r^3\right)}{a^3} = \frac{\left(\frac{16}{3} \pi r^3\right)}{\left(2\sqrt{2}r\right)^3} = \frac{\sqrt{2}\pi}{6} = 0.742$$

Ex. Al, Ag, Au, Cu

$$c^2 = a^2 + b^2$$

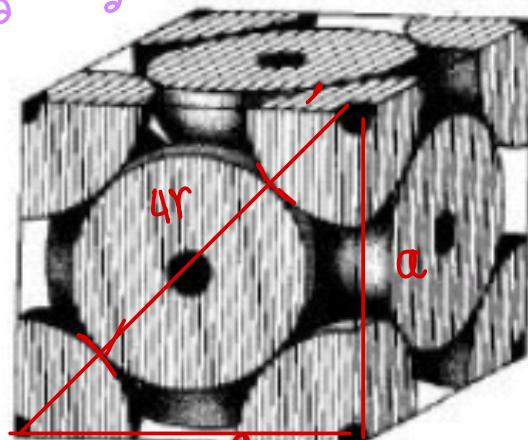
$$(4r)^2 = a^2 + a^2$$

$$16r^2 = 2a^2$$

$$\sqrt{16r^2} = \sqrt{2a^2}$$

$$4r = \sqrt{2}a$$

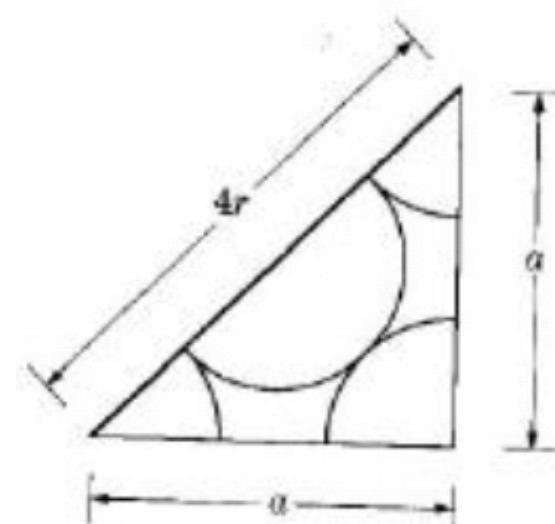
$$a = \frac{4r}{\sqrt{2}} \cdot \frac{\sqrt{2}}{\sqrt{2}} = \frac{4r\sqrt{2}}{2} = 2r\sqrt{2}$$



ຮັບຄວາມສ້າງແສດ້ນ

4 atoms in one unit cell.

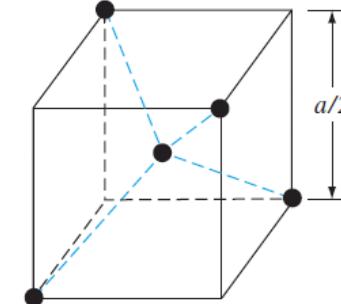
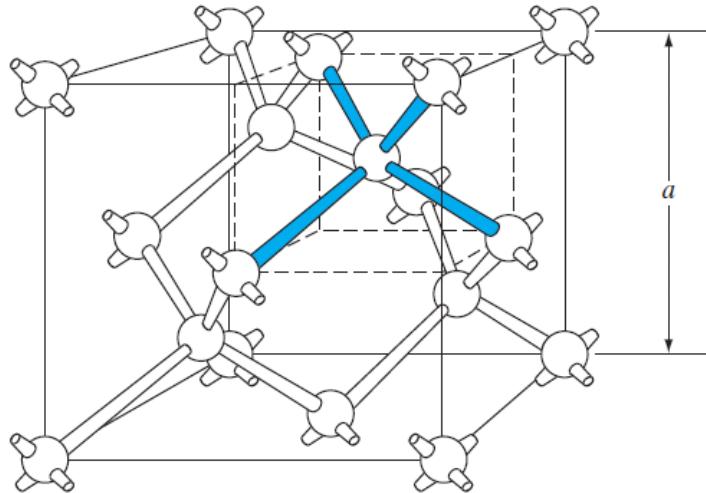
$$a = 2R\sqrt{2}$$



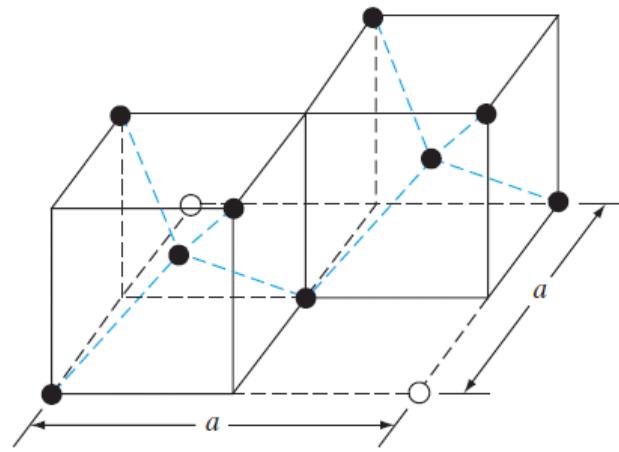
# *The Diamond Structure*

- This structure is like the FCC crystal family.
- It results from the interpenetration of two FCC lattices with one displaced from the other by one-quarter of the distance along a body diagonal of the cube or a displacement of  $a\sqrt{3}/4$

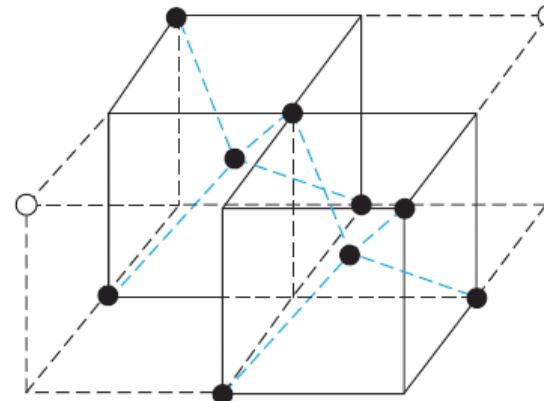
# *The Diamond Structure*



The tetrahedral structure of closest Neighbors in the diamond lattice.



(a)



(b)

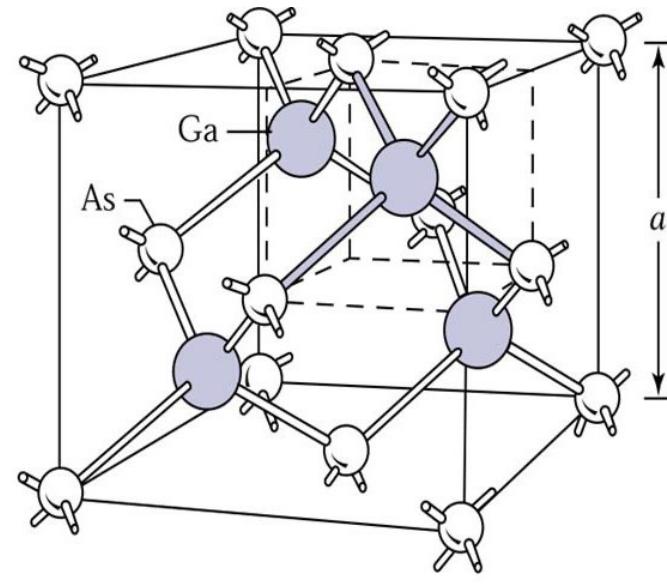
Portions of the diamond lattice: (a) bottom half and (b) top half.

# *The Diamond Structure*

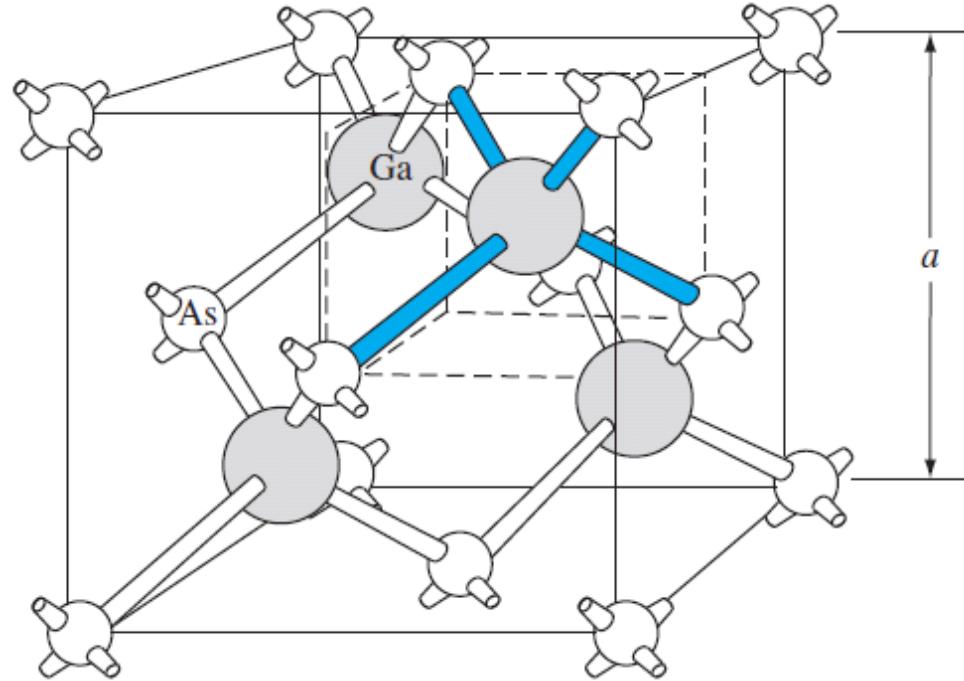
- If a corner atom has one nearest neighbor in the body diagonal, then it will have no nearest neighbor in the reverse direction.
- Therefore, there are eight atoms in one unit cell.
- Examples for this structure are Si and Ge.

# Zinc blende structure

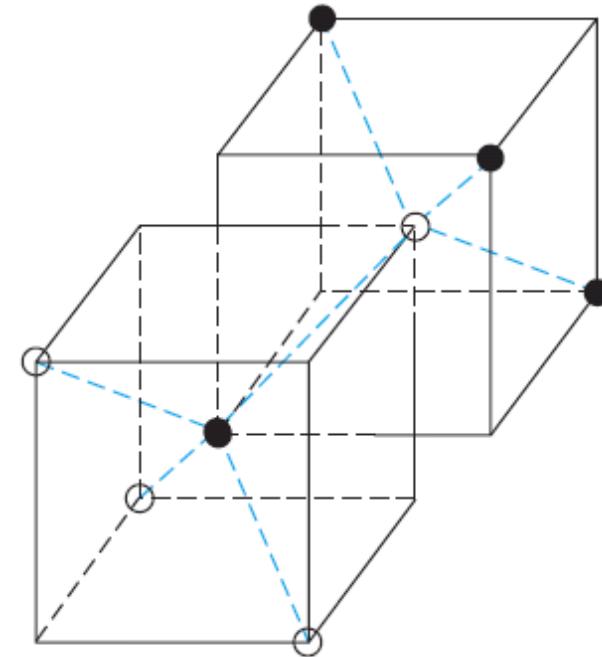
- For the Zinc blende structure, this results from the diamond structure with mixed atoms such that one FCC sublattice has column III (or V) atoms and the other has Column V (or III) atoms.
- This is a typical structure of III-V compounds.



Ex. GaAs, GaP, ZnS, CdS



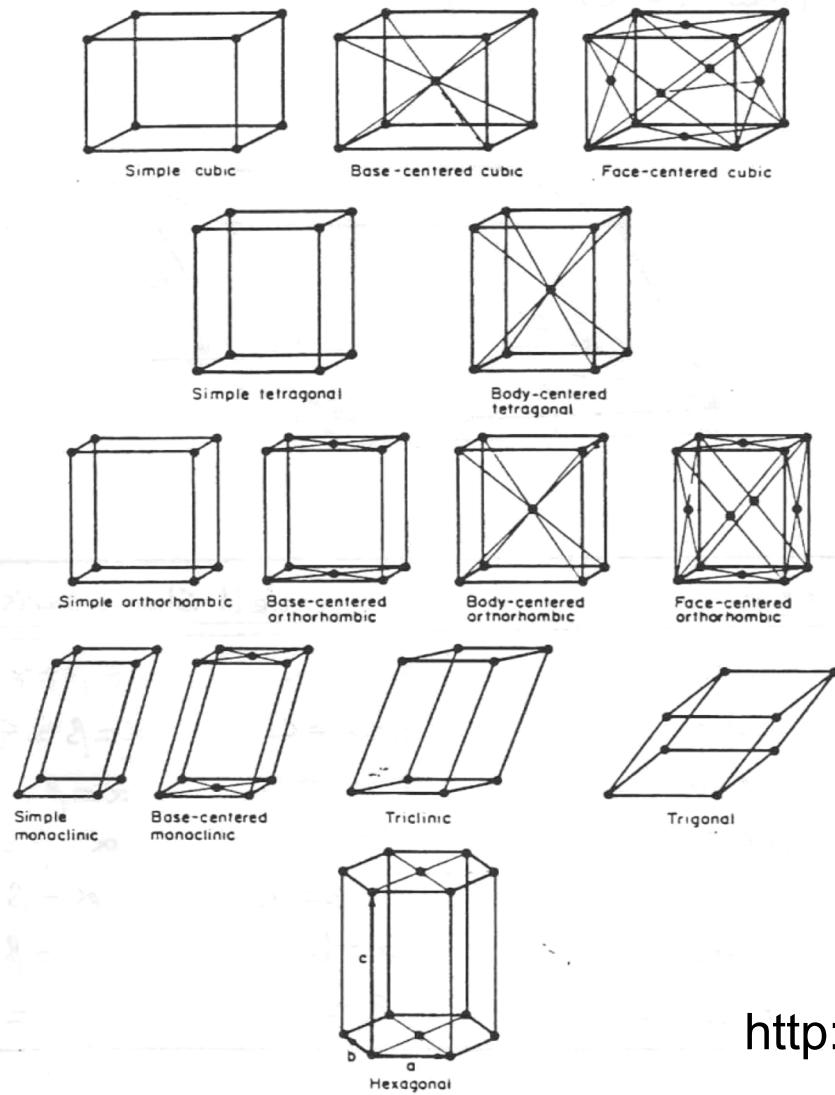
The zincblende (sphalerite) lattice of GaAs.



The tetrahedral structure of closest Neighbors in the zincblende lattice.

# Fourteen Bravais lattices

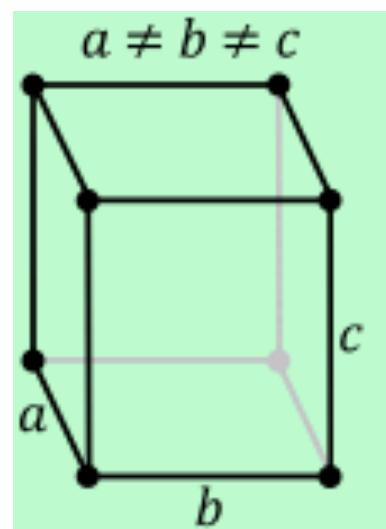
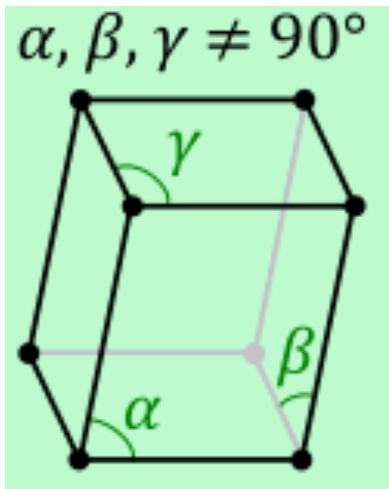
14 66909



- There are only 14 possible ways in 3-D space where lattice points could be arranged and each lattice points end up with some surroundings. This combination is called “**Bravais Lattices**”.

[http://en.wikipedia.org/wiki/Crystal\\_structure](http://en.wikipedia.org/wiki/Crystal_structure)

# Lattice systems



Lattice System	Unit cell properties
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
Trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$

# Crystal Planes and Miller Indices

- The crystal properties along different planes are different.
- The device characteristics (not only mechanical properties but also electrical properties) are dependent on the crystal orientation.
- The way to define crystal planes is to use ***Miller indices***.
- The Miller indices are useful to specify the orientation of crystal planes and directions.

# Crystal Planes and Miller Indices

There are some other conventions as:

1. **(hkl)**: For a plane that intercepts the negative x-axis, for example,  $(\bar{1}00)$
2. **{hkl}**: For planes of equivalent symmetry depending only on the orientation of the axes, e.g.  $\{100\}$  for  $(100)$ ,  $(010)$ ,  $(001)$ ,  $(0\bar{1}0)$ ,  $(00\bar{1})$ , and  $(\bar{1}00)$

# Crystal Planes and Miller Indices

3. **[hkl]**: For a crystal direction, such as [010] for the y-axis. By definition, the [010] direction is normal to (010) plane, and the [111] direction is perpendicular to the (111) plane.
4. **<hkl>**: For a full set of equivalent directions, e.g. <100> for [100], [010], [001],  $[\bar{1}00]$ ,  $[0\bar{1}0]$ , and  $[00\bar{1}]$ .

# Crystal Planes and Miller Indices

Miller indices can be obtained using this following procedure:

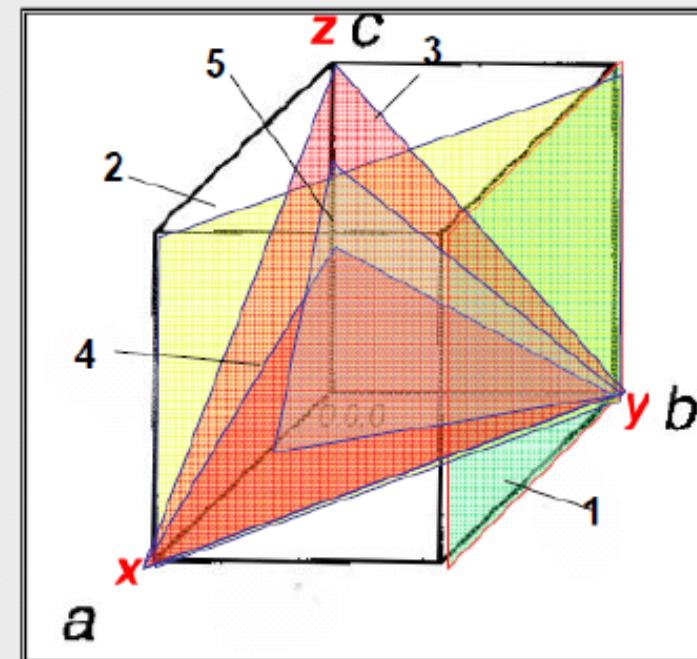
1. Determine the intercepts of the plane with crystal axes (three Cartesian coordinates).  
ນາງຄតຕົວແກນນັ້ນ
2. Take the reciprocals of the numbers from 1.  
ຕຳສ່ວນກົບ
3. Multiply the fractions by the least common multiple of the intercepts.  
ຈຳຄະນຸ້ນ
4. Label the plane in parentheses ( $hkl$ ) as the Miller indices for a single plane.  
ແຫຼ່ງເສີ່ງ

	x	y	z
①	3	2	4
②	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{4}$
③	$\frac{4}{12}$	$\frac{6}{12}$	$\frac{3}{12}$
④	4	6	3

	Intercept on axes	x (a)	y (b)	z (c)
	Reciprocal	1	1	$\frac{1}{2}$
	Integer Clear	1	1	2
	Miller Indices	$(112)$		
	Intercept on axes	x (a)	y (b)	z (c)
	Reciprocal	1	$\frac{3}{4}$	$\frac{1}{4}$
	Integer Clear	3	4	12
	Miller Indices	$\frac{1}{1} \frac{4}{3} \frac{4}{1}$	$(3 \ 4 \ 12)$	$\frac{3}{4} \frac{4}{12}$
	Intercept on axes	x (a)	y (b)	z (c)
	Reciprocal	1	1	$\infty$
	Integer Clear	1	1	0
	Miller Indices	$(110)$		

## Miller Indices-- Based on reciprocal of the intersection of the plane with the cell axes, indicated with parenthesis $(h, k, l)$

- Plane 1  $1/\infty, 1/1, 1/\infty = (010)$
- Plane 2  $1/1, 1/1, 1/\infty = (110)$
- Plane 3  $1/1, 1/1, 1/1 = (111)$
- Plane 4  $1/1, 1/1, 1/(1/2) = (112)$
- Plane 5  $1/(1/2), 1/1, 1/(1/4) = (634)$



-- Parallel planes have the same value  $(111) = (222)$

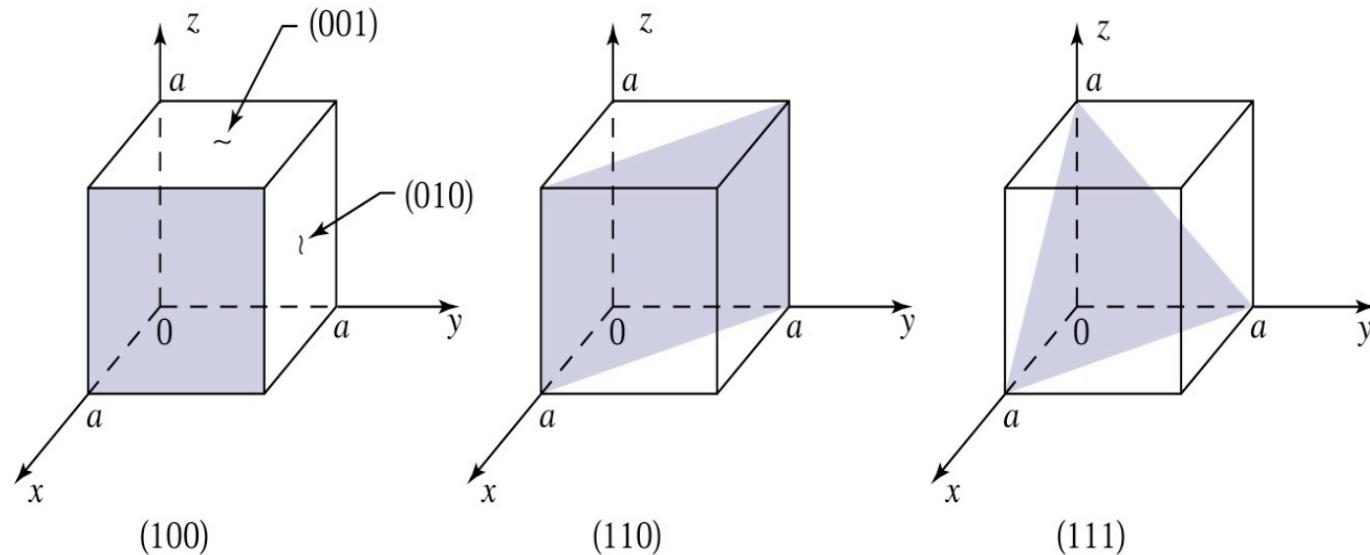
-- No Fractions, convert to integers  $(\frac{1}{2} \frac{1}{2} 1) = (112)$

-- Negative Direction has a top bar on the hkl value  $(1\bar{1}\bar{1})$

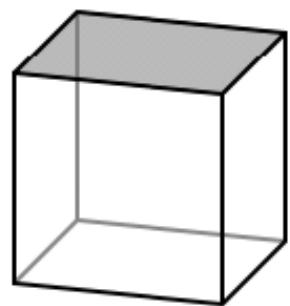


William H. Miller, 1801-1880,  
Professor of Mineralogy,  
Cambridge

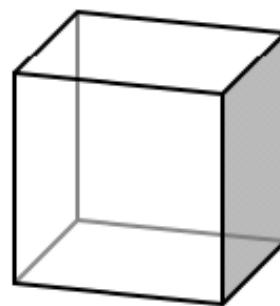
# Crystal Planes and Miller Indices



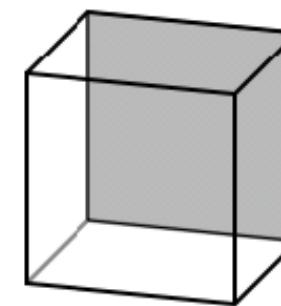
- The Miller indices of important planes in a cubic crystal.



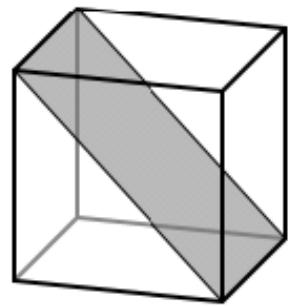
(001)



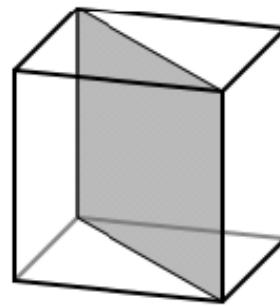
(100)



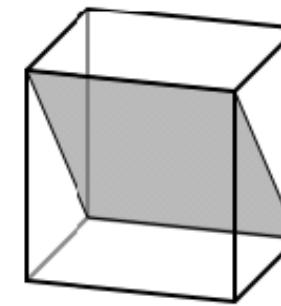
(010)



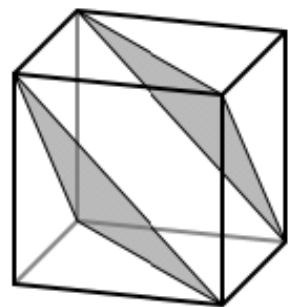
(101)



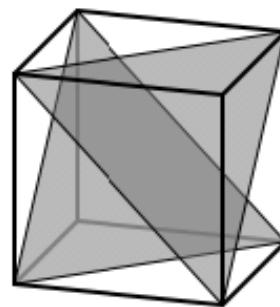
(110)



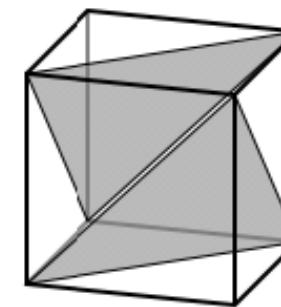
(011)



(111)



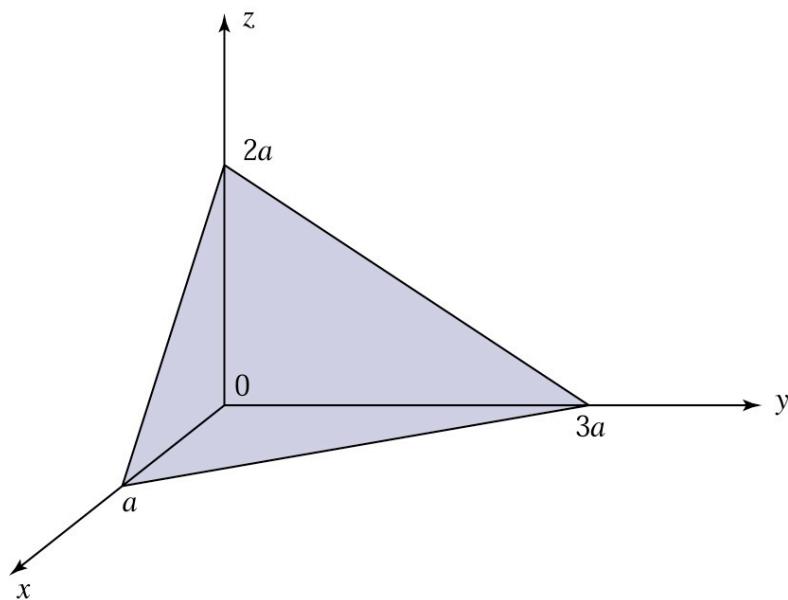
(1̄1̄1)



(1̄1̄1̄)

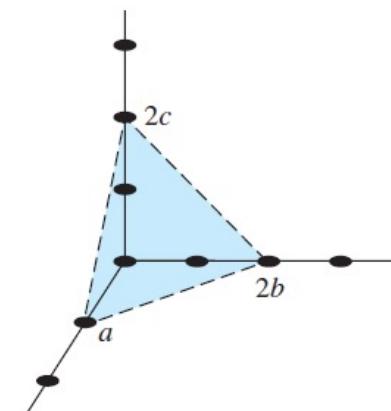
# Example 2

- Find the Miller indices of the below plane.



## EXERCISE PROBLEM

**Ex 1.2** Describe the lattice plane shown in Figure 1.7. (Ans. (211) plane)



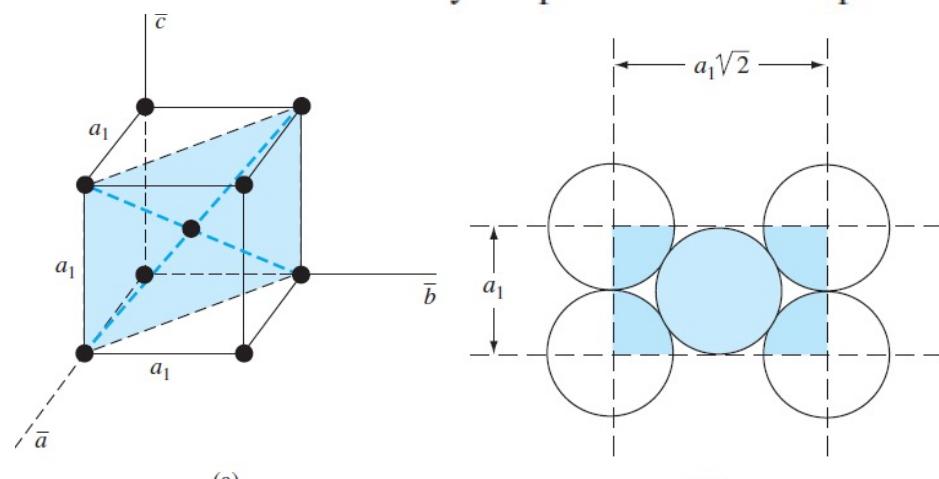
**Figure 1.7** | Figure for Exercise Problem Ex 1.2.

## Example 3

**Objective:** Calculate the surface density of atoms on a particular plane in a crystal.

Consider the body-centered cubic structure and the (110) plane shown in Figure 1.9a. Assume the atoms can be represented as hard spheres with the closest atoms touching each other. Assume the lattice constant is  $a_1 = 5 \text{ \AA}$ . Figure 1.9b shows how the atoms are cut by the (110) plane.

The atom at each corner is shared by four similar equivalent lattice planes, so each corner atom effectively contributes one-fourth of its area to this lattice plane as indicated in the figure. The four corner atoms then effectively contribute one atom to this lattice plane. The atom in the center is completely enclosed in the lattice plane. There is no other equivalent plane that cuts the center atom and the corner atoms, so the entire center atom is included in the number of atoms in the crystal plane. The lattice plane in Figure 1.9b, then, contains two atoms.



### ■ Solution

The number of atoms per lattice plane is  $\frac{1}{4} \times 4 + 1 = 2$

The surface density of atoms is then found as

$$\text{Surface Density} = \frac{\# \text{ of atoms per lattice plane}}{\text{area of lattice plane}}$$

So

$$\begin{aligned}\text{Surface Density} &= \frac{2}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5 \times 10^{-8})^2\sqrt{2}} \\ &= 5.66 \times 10^{14} \text{ atoms/cm}^2\end{aligned}$$

**Figure 1.9** | (a) The (110) plane in a body-centered cubic and (b) the atoms cut by the (110) plane in a body-centered cubic.

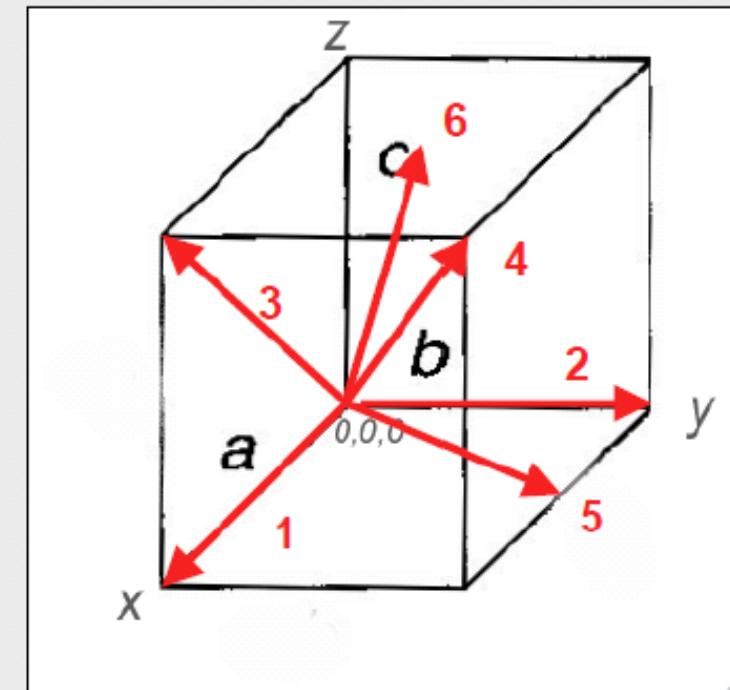
- Directions

**Based on intersection with the cell boundaries**

Indicated with square brackets [  $h, k, l$  ]

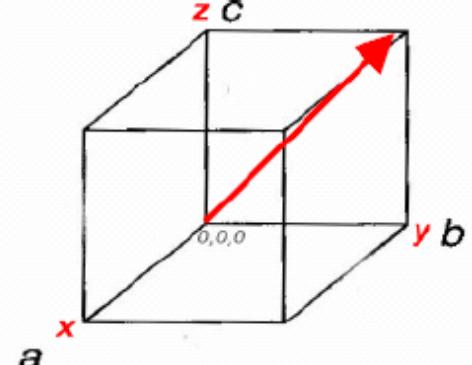
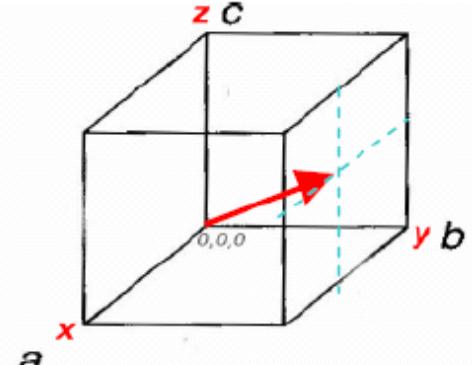
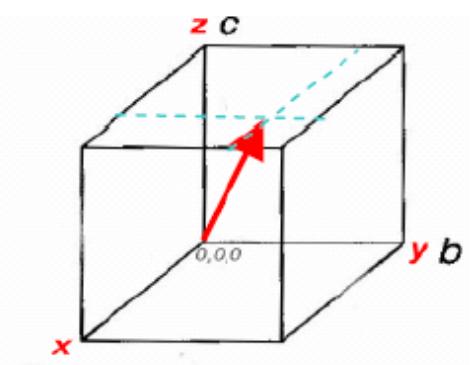
- Direction 1       $1, 0, 0 = [100]$
- Direction 2       $0, 1, 0 = [010]$
- Direction 3       $1, 0, 1 = [101]$
- Direction 4       $1, 1, 1 = [111]$
- Direction 5       $\frac{1}{2}, 1, 0 = [120]$
- Direction 6       $\frac{1}{2}, \frac{1}{2}, 1 = [112]$

-- Parallel directions have the same value  
Lowest Integer Value  $[111] = [222]$

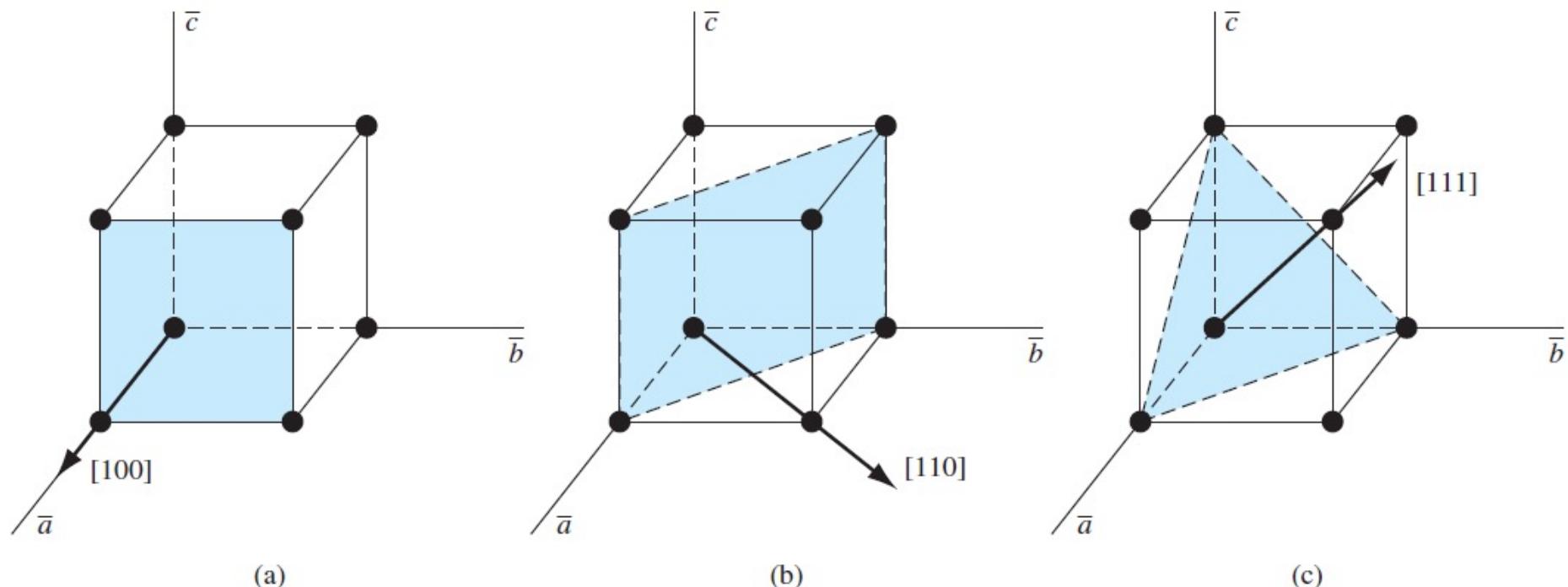


-- No Fractions, Convert to Integers  $[\frac{1}{2} \frac{1}{2} 1] = [112]$

-- Negative Direction has a top bar on the hkl value  $[1\bar{1}\bar{1}]$

	x (a)	y (b)	z (c)
Point Coordinates	0	1	1
Clear Fractions	0	1	1
Crystal Direction	[011]		
	x (a)	y (b)	z (c)
Point Coordinates	$\frac{1}{2}$	1	$\frac{1}{2}$
Clear Fractions	1	2	1
Crystal Direction	[121]		
	x (a)	y (b)	z (c)
Point Coordinates	$\frac{3}{4}$	$\frac{3}{4}$	1
Clear Fractions	3	3	4
Crystal Direction	[334]		

## Directions in Crystals



**Figure 1.10** | Three lattice directions and planes: (a) (100) plane and [100] direction, (b) (110) plane and [110] direction, (c) (111) plane and [111] direction.

# Density of crystal

- Crystal with a lattice constant “ $a$ ” and “ $n$ ” atoms within unit cell, then the weight of unit cell is equal to the weight of atoms per unit cell.
- The density of the crystal will be expressed as

$$\rho = \left( \frac{nM}{N_A} \right) \cdot \frac{1}{a^3}$$

จำนวนอะตอม  $\downarrow$  น้ำหนักของอะตอม (มวล relative)  
ค่าอนุกรมน้ำหนักเฉลี่ย  $\rightarrow$  รูปแบบที่ใช้กว้างๆ อะตอมมากทำส่วนกลับ  $\uparrow$   
 $\rightarrow$  เลข ๖.๐๒๒ โคลัมเบิร์ก  $\uparrow$   $6.022 \times 10^{23}$

where

$\rho$  = density of crystal [g/cm<sup>3</sup>]

$M$  = atomic weight [g/mole]

$N_A$  = Avogadro's number =  $6.022 \times 10^{23}$  atoms/mole

$n/a^3$  = number of atoms per unit volume

# Example 1

**Objective:** Find the volume density of atoms in a crystal.

Consider a single-crystal material that is a body-centered cubic, as shown in Figure 1.5b, with a lattice constant  $a = 5 \text{ \AA} = 5 \times 10^{-8} \text{ cm}$ . A corner atom is shared by eight unit cells that meet at each corner so that each corner atom effectively contributes one-eighth of its volume to each unit cell. The eight corner atoms then contribute an equivalent of one atom to the unit cell. If we add the body-centered atom to the corner atoms, each unit cell contains an equivalent of two atoms.

$$a: 5 \text{ \AA}: 5 \times 10^{-8} \text{ cm}: 5 \times 10^{-10} \text{ m}$$

## ■ Solution

The number of atoms per unit cell is  $\frac{1}{8} \times 8 + 1 = 2$

atoms

The volume density of atoms is then found as

$$\text{Volume Density} = \frac{\# \text{ atoms per unit cell}}{\text{volume of unit cell}}$$

So

$$\text{Volume Density} = \frac{2}{a^3} = \frac{2}{(5 \times 10^{-8})^3} = 1.6 \times 10^{22} \text{ atoms/cm}^3$$

## ■ EXERCISE PROBLEM

**Ex 1.1** The lattice constant of a face-centered cubic lattice is 4.25 Å. Determine the  
(a) effective number of atoms per unit cell and (b) volume density of atoms.

(Ans. (a) 4, (b)  $5.21 \times 10^{22} \text{ cm}^{-3}$ )

## Example 2

$$\begin{aligned} & 273 + {}^\circ\text{C} : \text{K} \\ & 273 + {}^\circ\text{C} : 300 \\ & \text{C} : 27^\circ\text{C} \end{aligned}$$

$$5.43 \times 10^{-8} \text{ cm}$$

- At 300 K the lattice constant for Si is 5.43 Å. Calculate the number of Si atoms per cubic centimeter and the density of Si at room temperature. Note: Atomic weight of Si = 28.09 g/mole

$$\textcircled{1} \quad n = \frac{8}{(5.43 \times 10^{-8})^3} = 4.99 \times 10^{22} \text{ atoms/cm}^3$$

$$\textcircled{2} \quad \rho = \frac{nM}{N_A} \cdot \frac{1}{a^3} = \frac{5 \times 10^{22} \text{ atoms}}{6.022 \times 10^{23} \text{ atoms/mol}} \cdot \frac{28.09 \text{ g/mol}}{\text{mol}} = 2.33 \text{ g/cm}^3$$

## Example 3

- Find the density of Cu in [g/cm<sup>3</sup>]. Cu has an atomic radius of 1.278 Å and atomic weight of 63.5 g/mole.