

# Crystal Structure and Defects

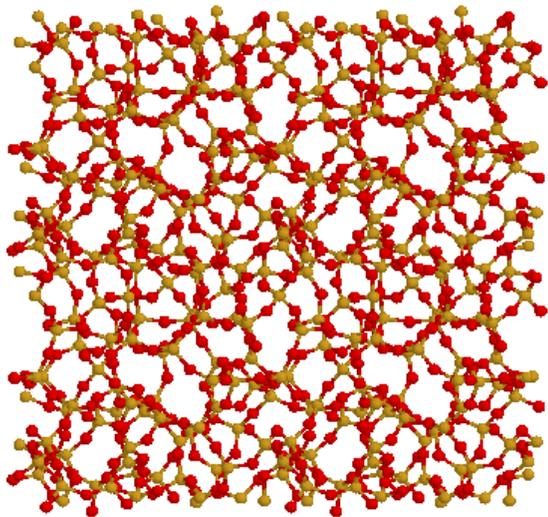
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- The goal of this lecture is to review some fundamental concepts from Materials Science necessary to understand and to talk about the properties of the materials we are processing.
  - Microstructure
  - Crystal Structure and Crystallography
  - Crystal Defects

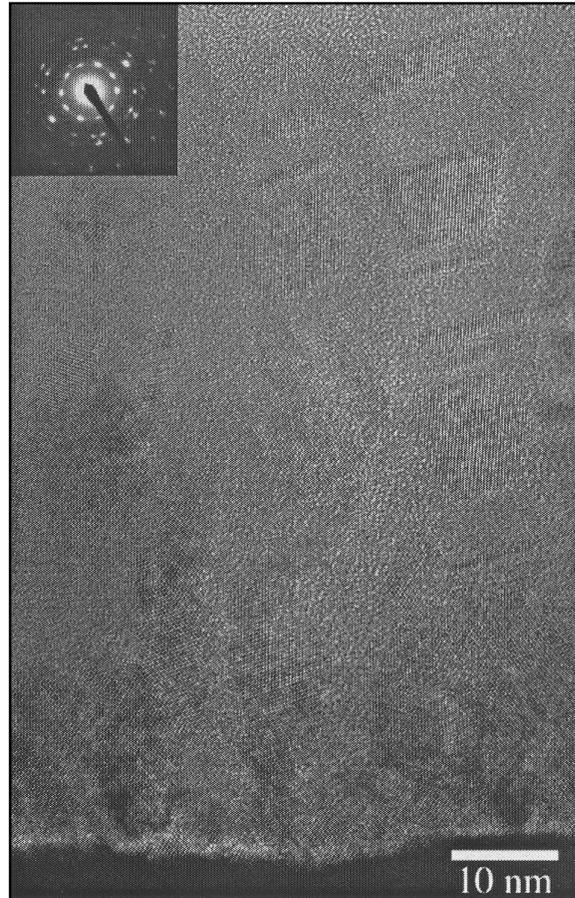




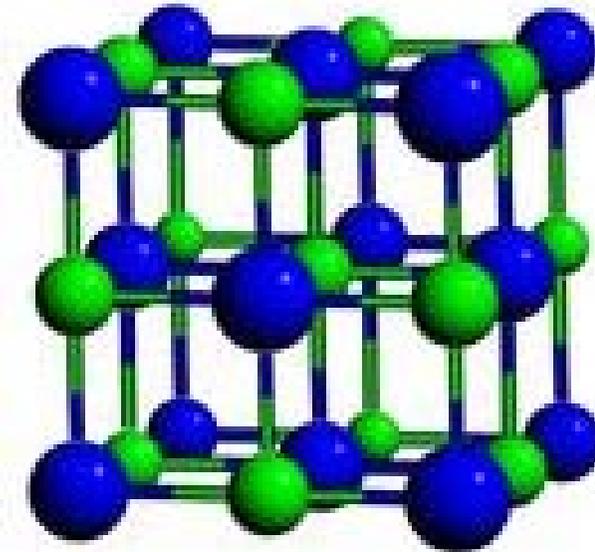
# Microstructure of Materials



Amorphous



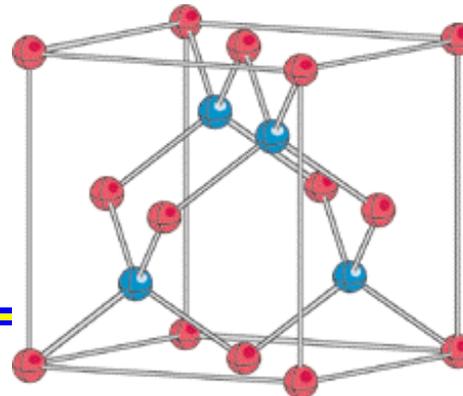
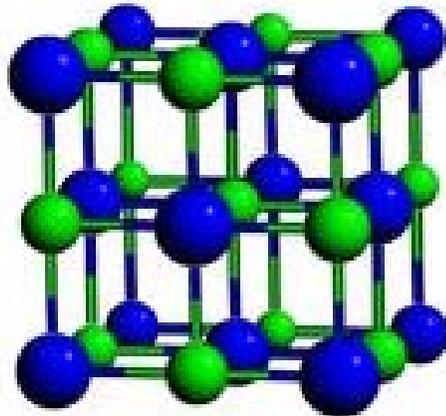
Polycrystalline



Crystalline

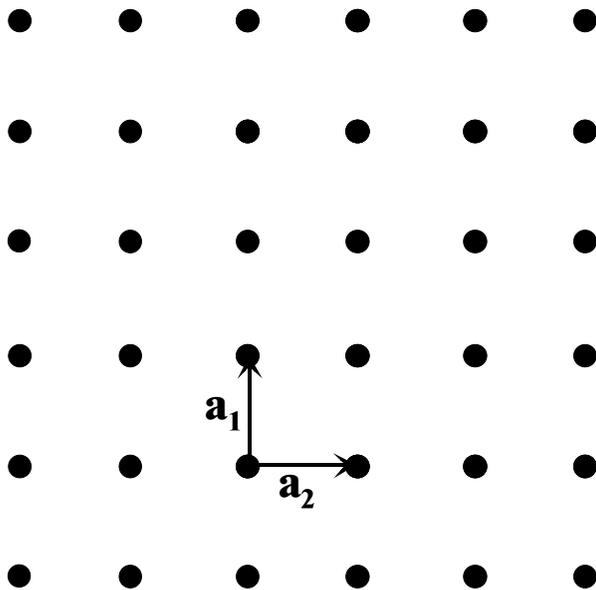
# Crystal Structure

- Crystal structures are regular 3-dimensional patterns of atoms in space
- The regularity with which atoms are packed in solids arises from geometrical conditions (i.e., bond angles and lengths) which are imposed by directional bonding and close packing
- Most stable arrangement will be the one that
  - 1) Minimizes energy/volume
  - 2) Preserves electrical neutrality
  - 3) Satisfies directionality and discreteness of the covalent bonds
  - 4) Minimizes ion-ion repulsion
  - 5) Packs atoms as closely as possible consistent with (1)-(5)



# Description of Crystal Structure: Lattice

- A **lattice** is an infinite three dimensional array of points in which every point has surroundings identical with that of every other point. These are called **lattice points**.
- Example: A 2-D square space lattice:



Set of all points  $\vec{r}'$  defined by

$$\vec{r}' = \vec{r} + u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3$$

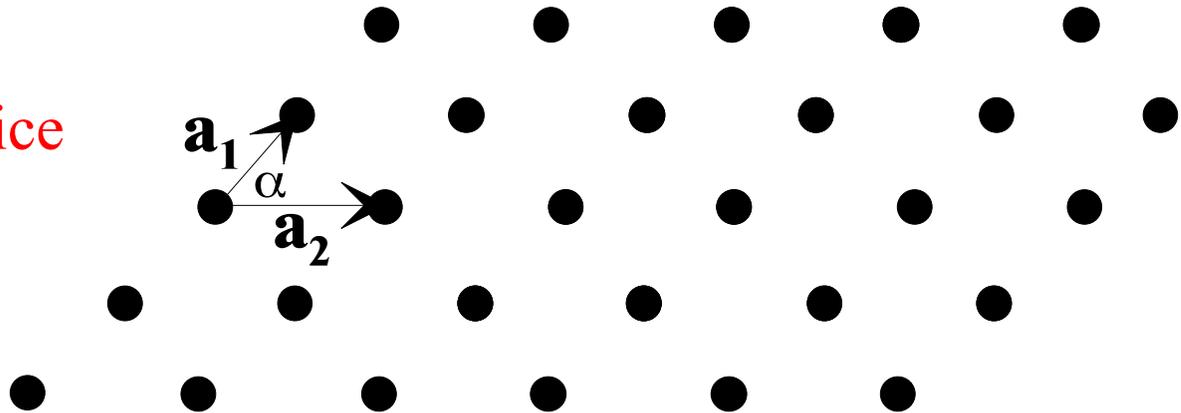
where  $u_1, u_2, u_3$  are integers



# Bravais Space Lattices

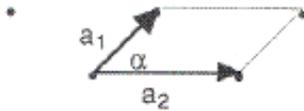
- The most general (“lowest symmetry”) 2-D lattice is the “oblique lattice” in 2-D.
- $a_1$  and  $a_2$  are called lattice translation vectors. Translation by integer multiple of  $a_1$  and  $a_2$  takes one from one lattice point to another
- There is an infinite number of lattices because there are no restrictions on the length or the angle ( $\alpha$ ) between the lattice translation vectors.
- But restrictions on the number of lattices are placed if relations between lengths of  $a_1$  and  $a_2$  and  $\alpha$  are specified

2-D Oblique lattice



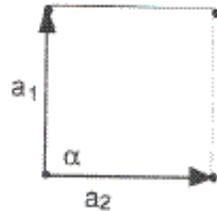
# Bravais Lattices in 2-D

- 4 restrictions that can be imposed on  $a_1, a_2$  and  $\alpha$  gives rise to total of 5 Bravais lattices in 2-D (1 general, 4 special lattices).



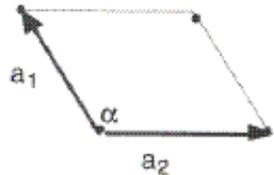
$$a_1 \neq a_2 \quad \alpha \neq 90 \text{ or } 120$$

Oblique lattice



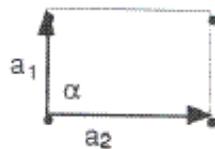
$$a_1 = a_2 \quad \alpha = 90$$

Square lattice



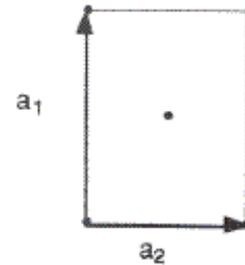
$$a_1 = a_2 \quad \alpha = 120$$

Hexagonal lattice



$$a_1 \neq a_2 \quad \alpha = 90$$

Rectangular lattice



$$a_1 \neq a_2 \quad \alpha = 90$$

Centered Rectangular Lattice

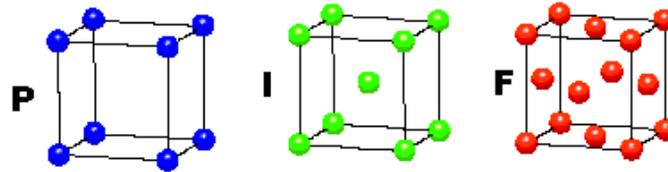


# 14 Bravais Space Lattices in 3-D

## CUBIC

$$a = b = c$$

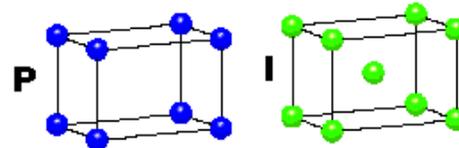
$$\alpha = \beta = \gamma = 90^\circ$$



## TETRAGONAL

$$a = b \neq c$$

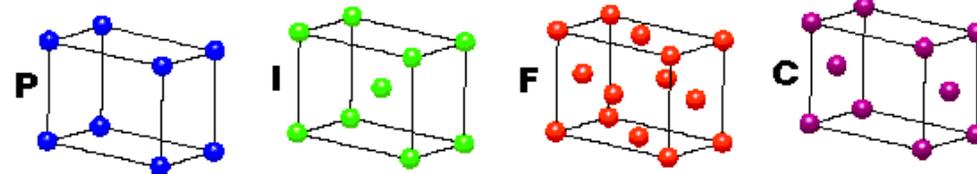
$$\alpha = \beta = \gamma = 90^\circ$$



## ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

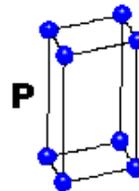


## HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

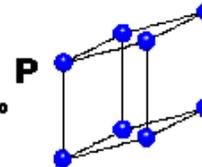
$$\gamma = 120^\circ$$



## TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

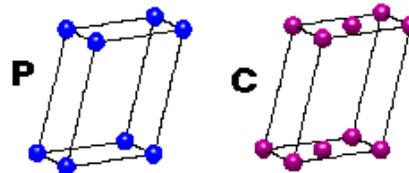


## MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

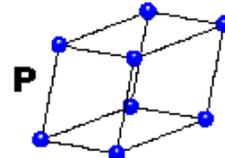
$$\beta \neq 120^\circ$$



## TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



### 4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

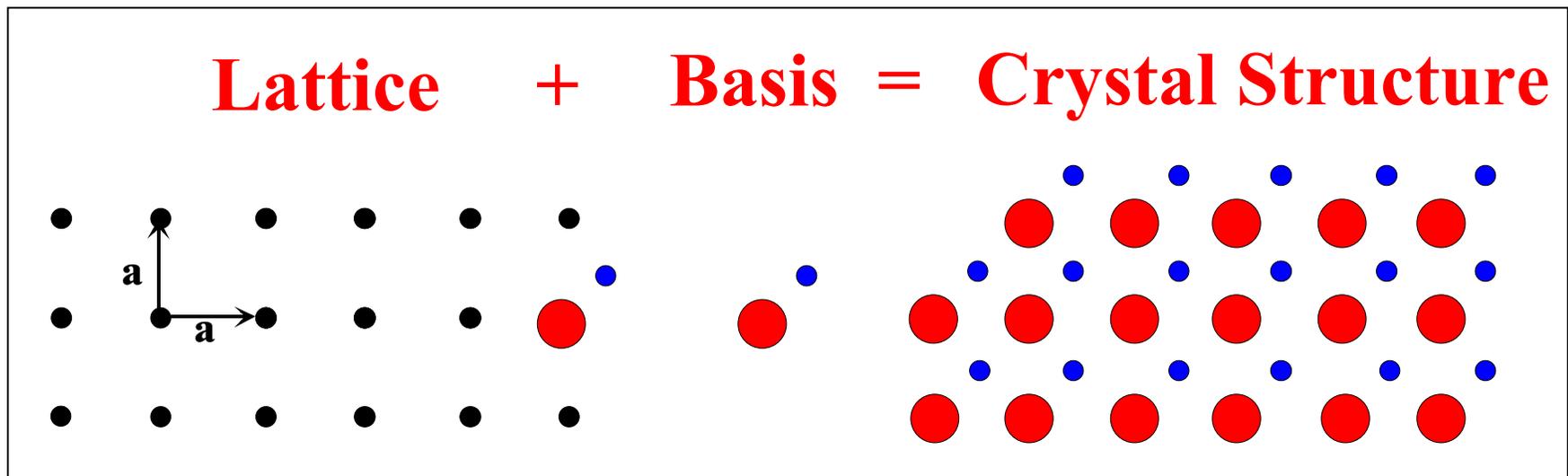
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7 Crystal Classes

→ 14 Bravais Lattices

# Specifying Crystal Structure

- A **motif** or a **basis** is a specific arrangement of atoms which belong to a lattice point.
- Crystal structure can be completely described by specification of a lattice and basis



Lattice is square lattice

Basis is large red atom at (0,0) and small blue atom at ( $\frac{1}{2} a$ ,  $\frac{1}{2} a$ )

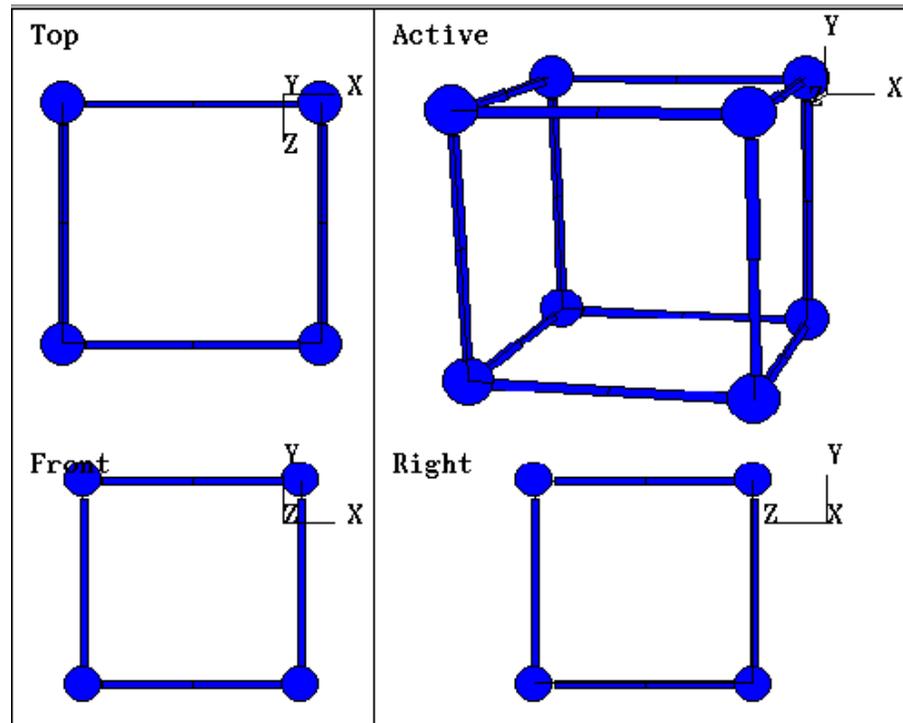


# Unit Cell

- Moving the basis from lattice point to lattice point generates a crystal structure.
- A **unit cell** is a repeating unit of the space lattice which can be used to reproduce the entire cell. Lattice + basis specifies a **unit cell**.
- Primitive unit cell is one that has only one atom per unit cell and the lattice vectors defining the cell are said to be primitive lattice vectors.
- We often use primitive translation vectors and unit cells to define the crystal structure but nonprimitive axes are also used when they have simpler relation to the symmetry of the structure.



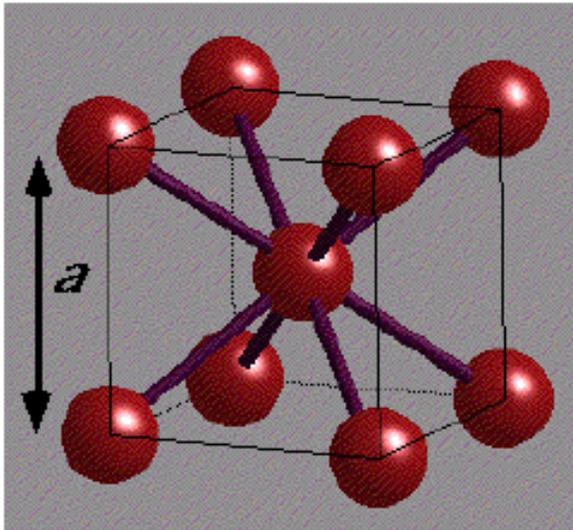
# Simple 3-D Unit Cells: Simple cubic (SC)



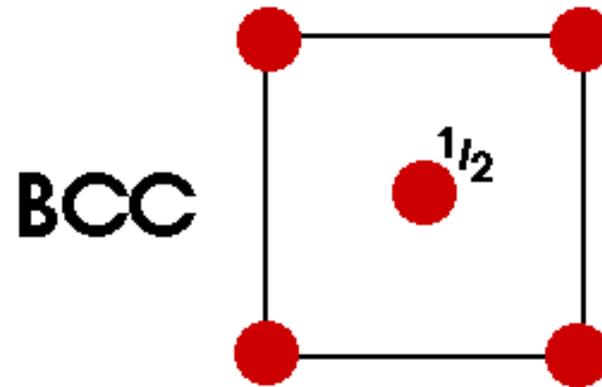
- 1 lattice points per cell
- Po crystal structure = SC lattice + 1 atom at lattice sites
- 6 nearest neighbors at a ( $a$  = lattice parameter)



# Simple 3-D Unit Cells: Body centered cubic (BCC)



## Body-Centred Cubic



- 2 lattice points per cell
- Mo, W crystal structure = BCC lattice + 1 atom at lattice sites
- 8 nearest neighbors at  $0.87 a$



# BCC Primitive Unit Cell

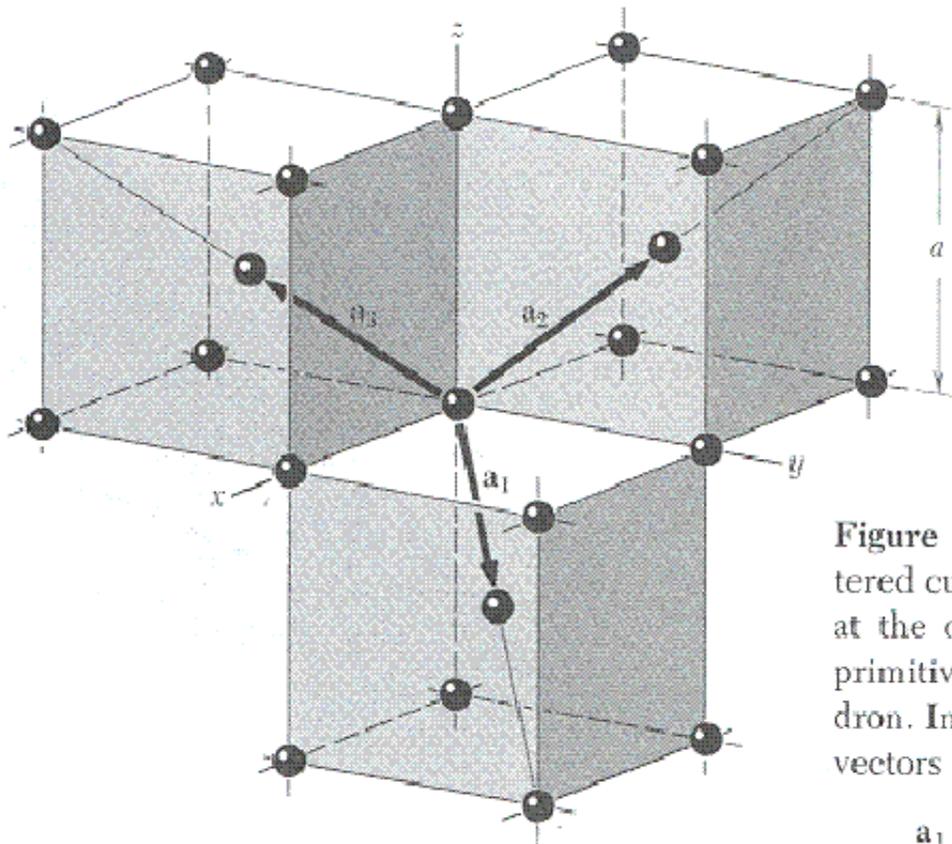
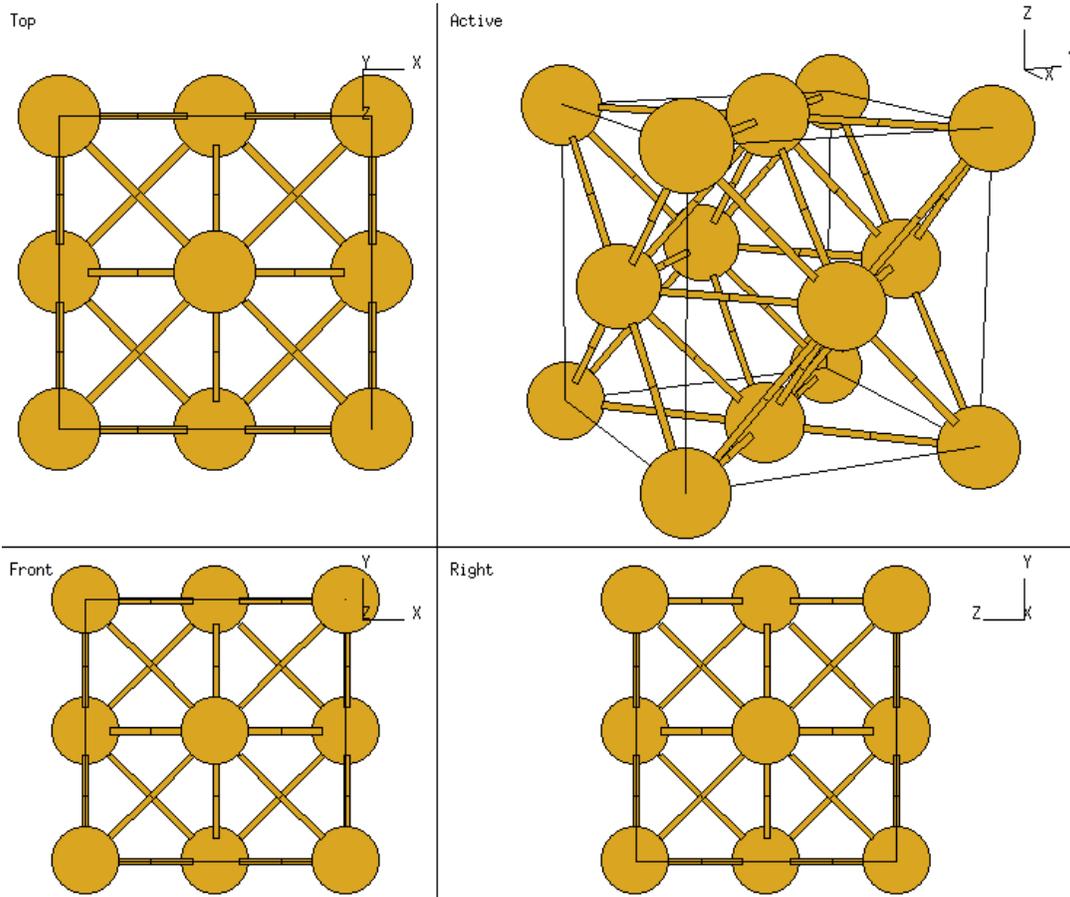


Figure 12 Primitive translation vectors of the body-centered cubic lattice; these vectors connect the lattice point at the origin to lattice points at the body centers. The primitive cell is obtained on completing the rhombohedron. In terms of the cube edge  $a$  the primitive translation vectors are

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z}) ; & \mathbf{a}_2 &= \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z}) ; \\ \mathbf{a}_3 &= \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z}) . \end{aligned}$$



# FCC Unit Cell and FCC Crystal Structure



- 4 lattice points per cell
- Cu, Au, Ag, Pt, etc. crystal structure = FCC lattice + 1 atom at lattice sites
- 12 nearest neighbors; close packed structure

<http://cst-www.nrl.navy.mil/lattice/>

<http://www.webelements.com/webelements/elements/text/Pt/xtal-vr.html>



# FCC Primitive Unit Cell

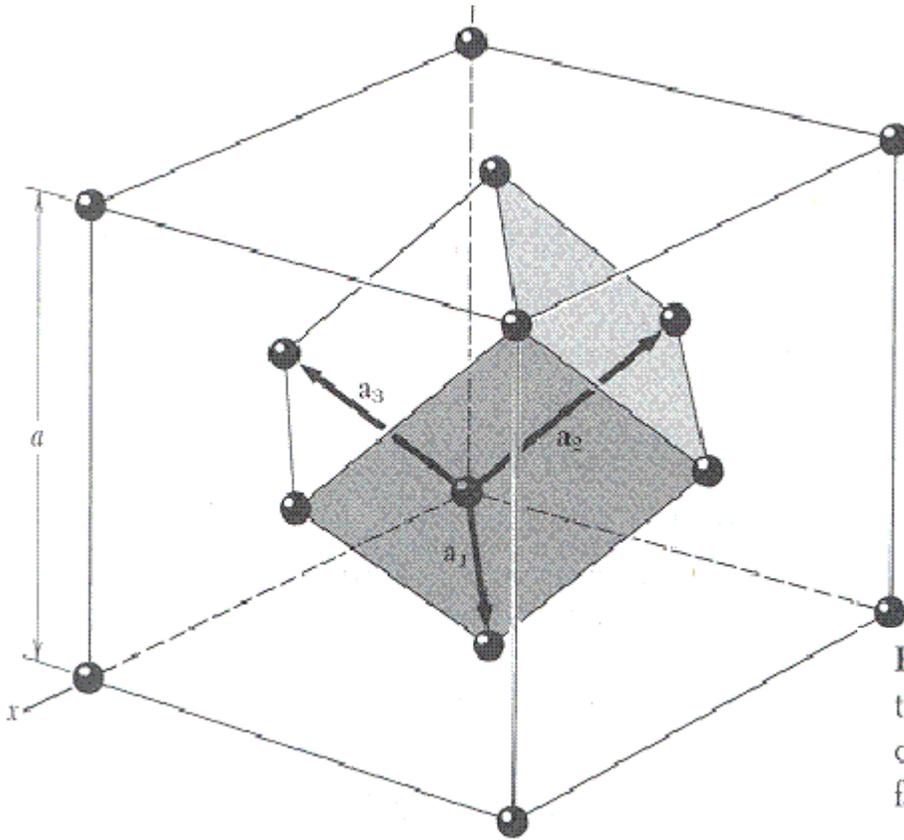


Figure 13 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$  connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

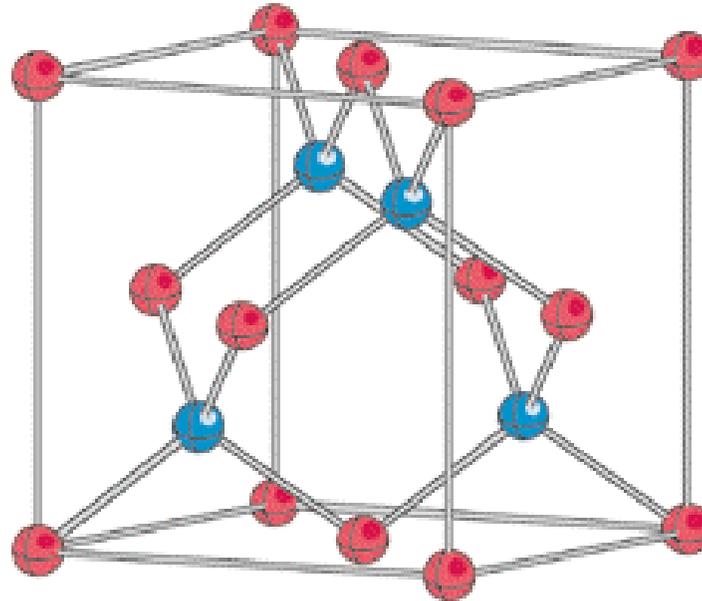
$$\mathbf{a}_1 = \frac{1}{2}a(\hat{x} + \hat{y}) ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{y} + \hat{z}) ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{z} + \hat{x}) .$$

The angles between the axes are  $60^\circ$ . Here  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{z}$  are the Cartesian unit vectors.



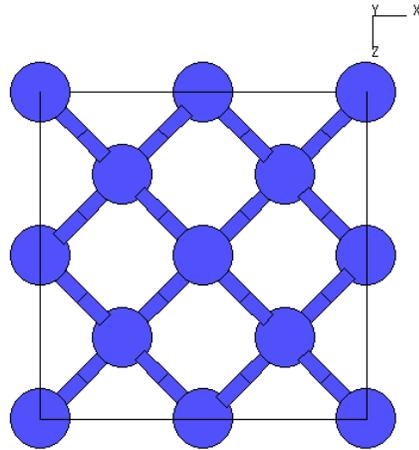
# The Diamond Lattice

- The crystal structure of group IV semiconductors (Si and Ge) is described by unit cell known as the diamond lattice unit cell
- Diamond structure is an FCC Bravais lattice with a basis that has two identical (e.g., Si, Ge, or C) atoms at each and of the vector  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$ , where  $a$  is the lattice constant (different for Si, Ge and C).

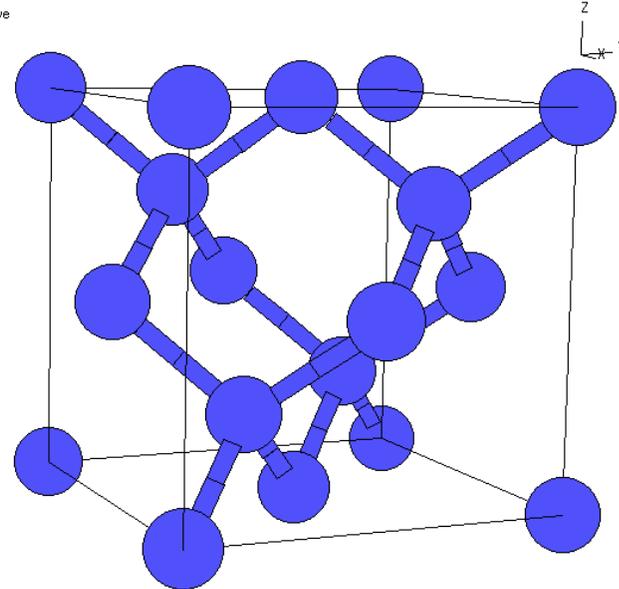


# Diamond Structure

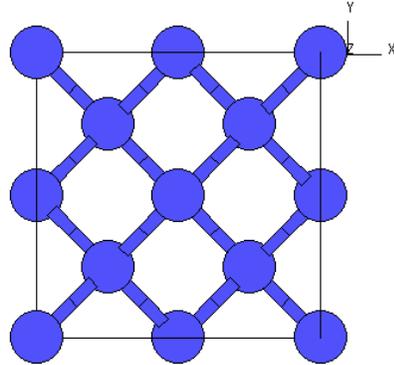
Top



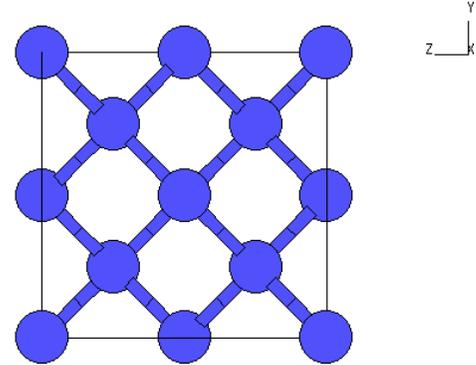
Active



Front

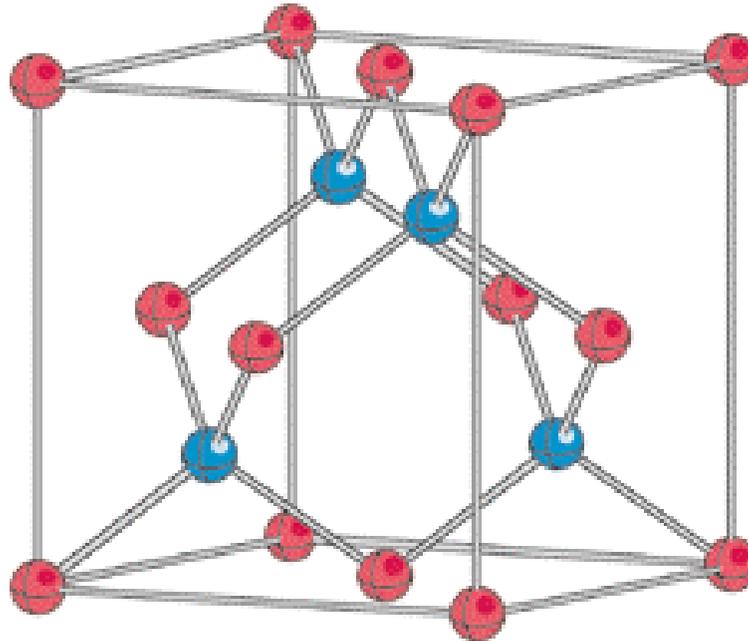


Right



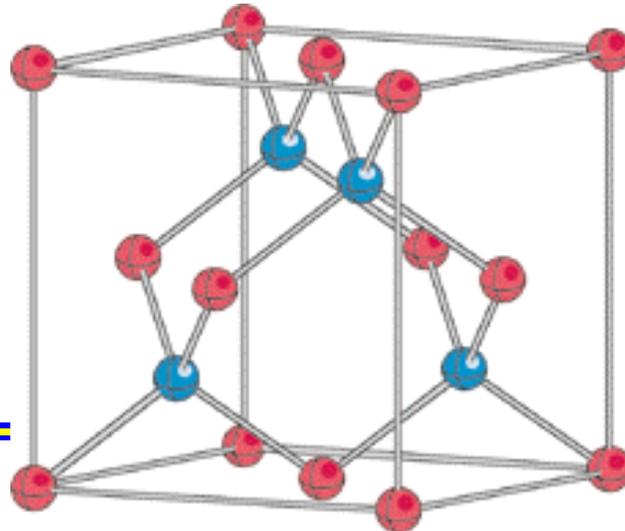
# The Diamond Lattice

- A less formal way of visualizing the diamond structure is to think of it in terms of two FCC lattices interpenetrating each other.
- One FCC lattice is shifted with respect to the other along the body diagonal by  $\frac{1}{4}$  of the body diagonal length



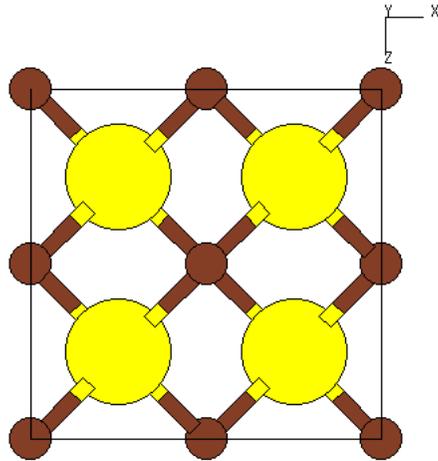
# The Zincblende Structure

- GaAs has the Zinc blende structure
- An FCC Bravais lattice with a basis that has two different atoms one at the each end of the vector  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$  (e.g., Ga on one end and As on the other end)
- Zincblende structure is the same as the diamond structure (*two FCC lattices interpenetrating each other with one FCC lattice shifted with respect to the other along the body diagonal by  $\frac{1}{4}$  of the body diagonal length*) but the two FCC lattices are made of different atoms

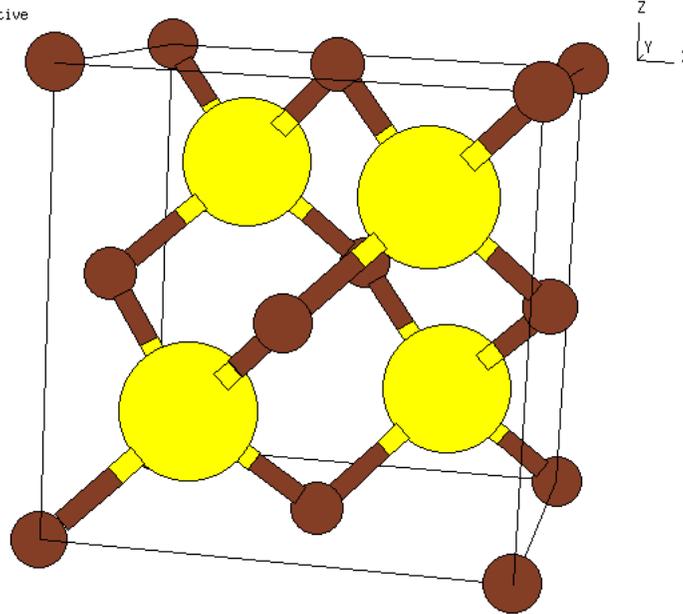


# The Zincblende Structure

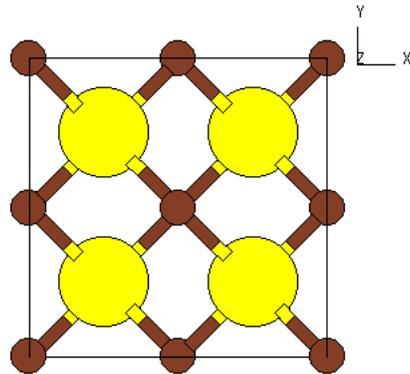
Top



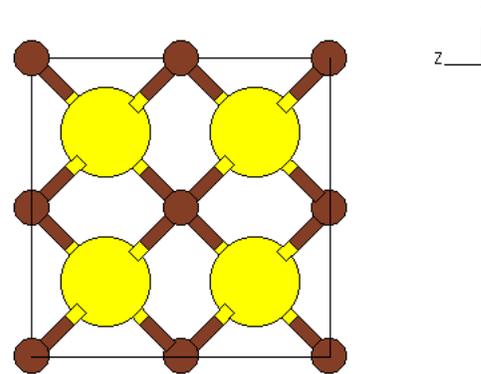
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Front



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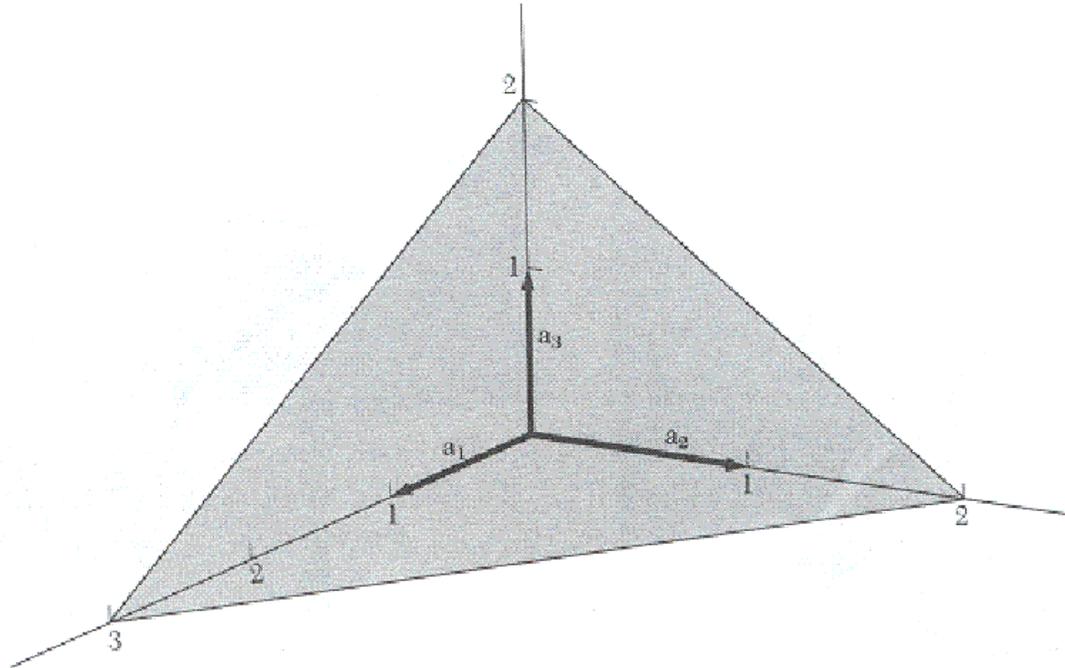


# Miller Indices

- Miller indices help specify atomic planes and orientations in a crystal
- To obtain Miller indices of any plane of atoms do the following.
  - 1) Set up coordinate axes along the edges of the unit cell and note where the plane in question intercepts the axes (x,y,z).
  - 2) Take the reciprocal of the intercepts.
  - 3) Using appropriate multiplier convert the reciprocals obtained to smallest set of whole numbers.
  - 4) By convention these numbers (h,k,l) are enclosed in () to identify a plane. If any of the numbers have a negative sign a bar is located at the top of that index.
- Equivalent planes (family of planes that contain identical atomic arrangements) are referenced by enclosing one of the members of the group in {}. e.g., in diamond structure  
 $\{001\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$



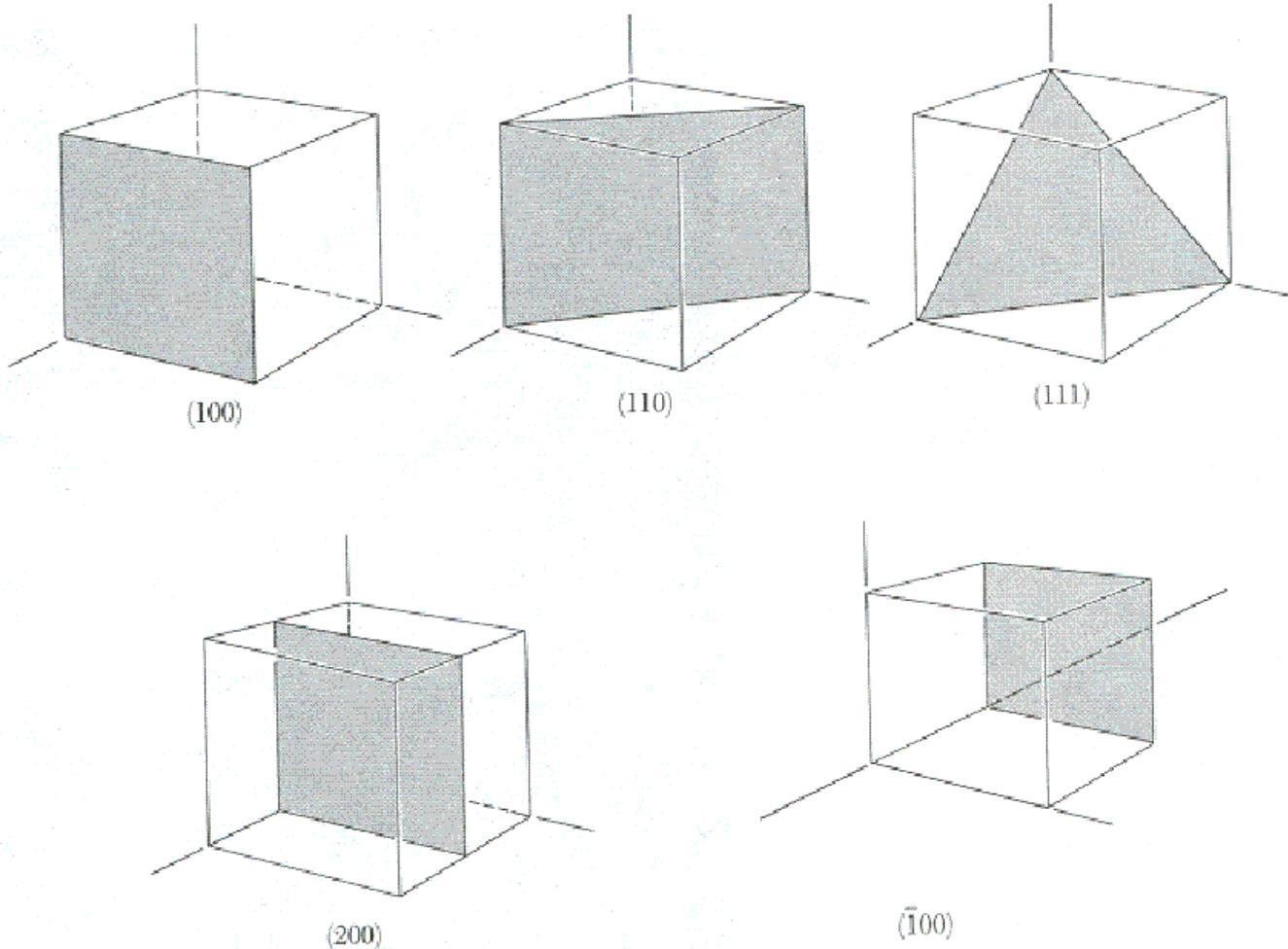
# Miller Indices Examples



- Plane intercepts x,y,z axes at  $3a_1$ ,  $2a_2$ , and  $2a_3$  respectively
- Reciprocals are  $1/3$ ,  $1/2$ , and  $1/2$
- To get smallest integers having this ratio multiply by common denominator 6. Thus this is the (233) plane



# Miller Indices Examples



# Crystallographic Directions

- Miller indices enclosed within [ ] are used to designate directions within a crystal
- Note also that the Miller indices also give the direction of the normal vector of the plane they describe
- Miller indices enclosed within < > are used to designate equivalent (family of) directions.

e.g., in simple cubic lattice [100] is the x-axis direction, <100> describes all directions parallel to the x, y and z axis.



# Crystal Defects

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- **Defects** are imperfections which cause disruption in what otherwise would be a perfect lattice.
- Defects are classified based on their dimensionality
  - Point defects (0-D)
  - Line defects (1-D)
  - Surface Imperfections (2-D)
  - Volume defects (3-D)

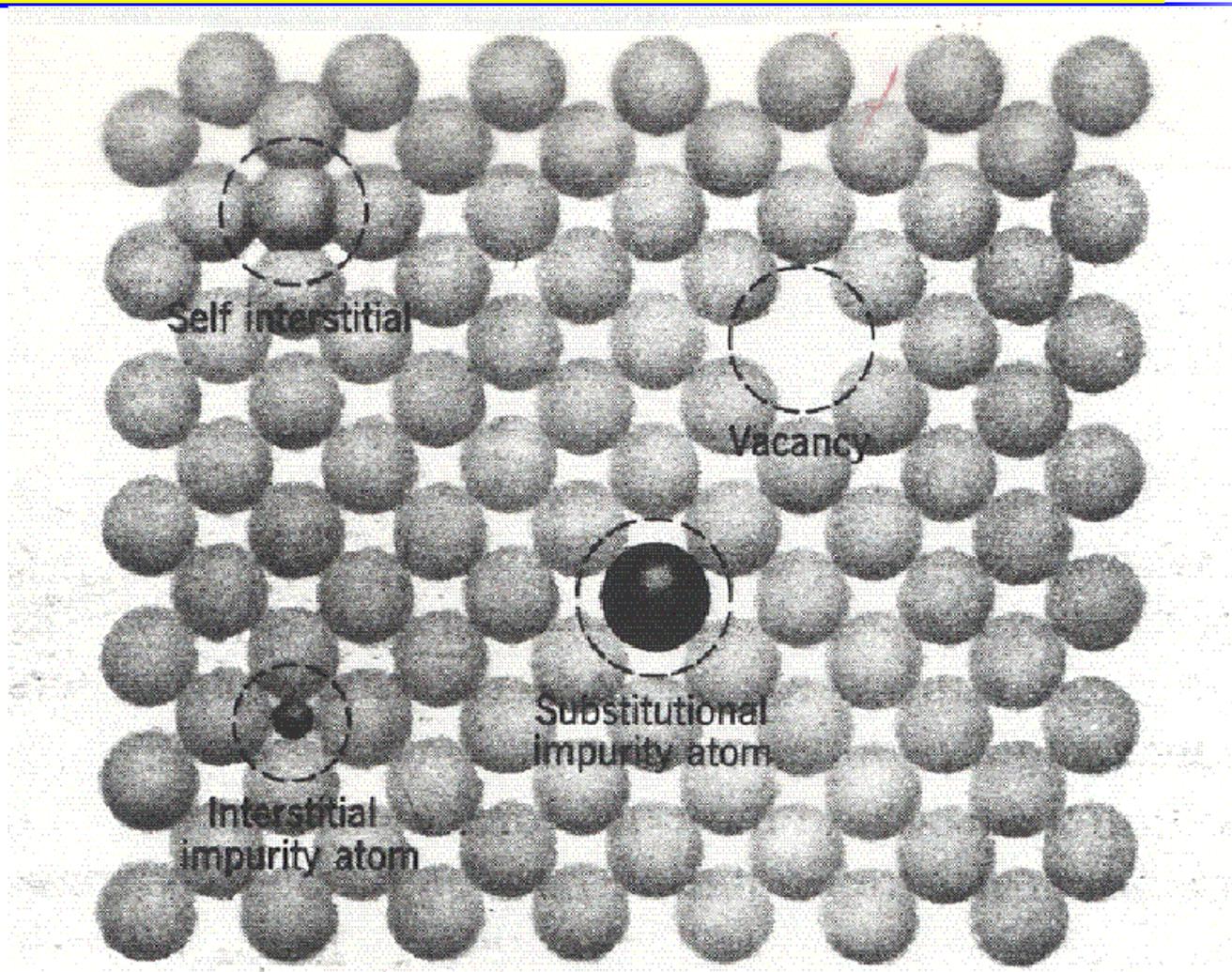


# Point Defects

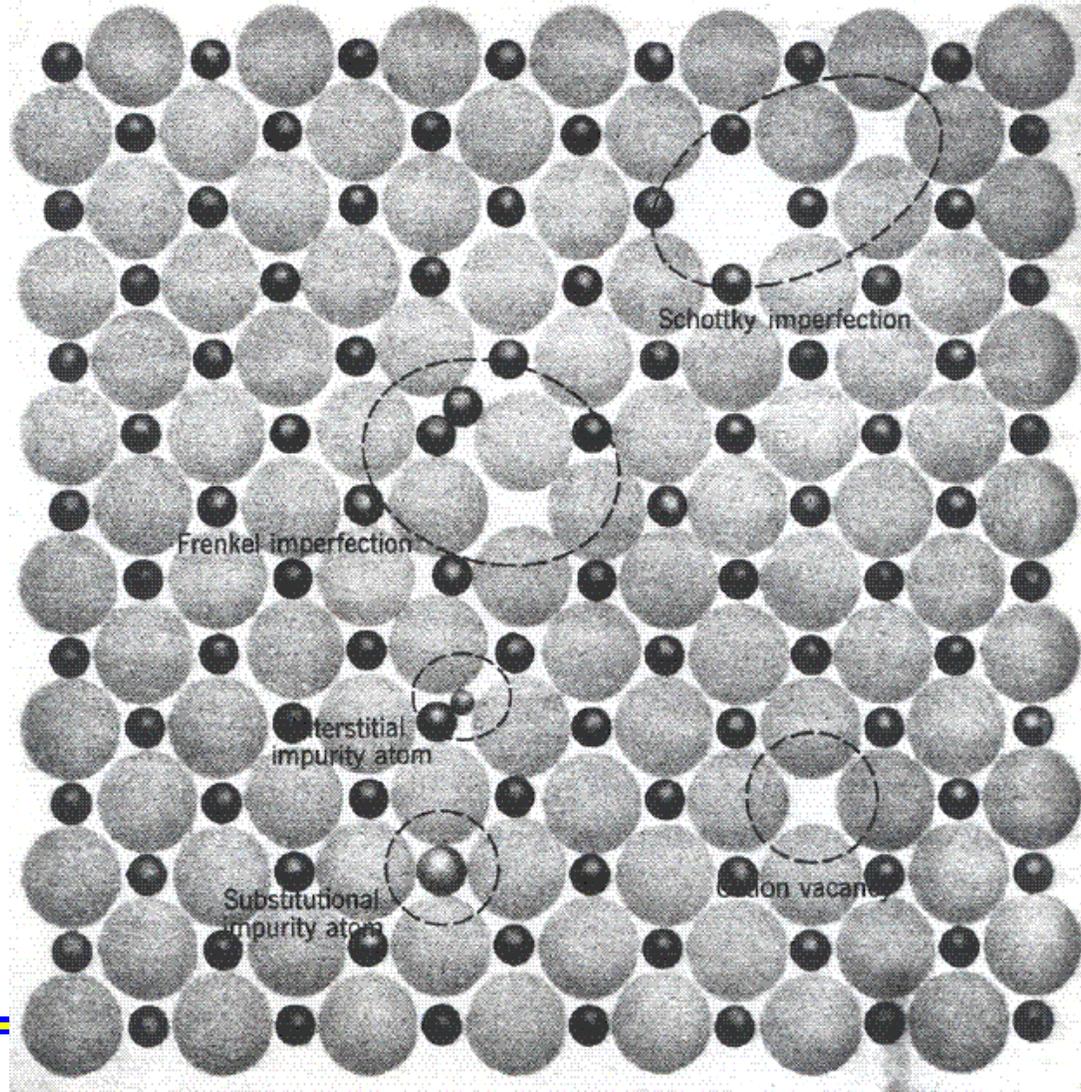
- **Vacancy:** absence of an atom in a lattice point where there is suppose to be an atom. Formed when atoms are removed from their lattice positions (typically to the surface) as a result of thermal fluctuations. AKA Schottky defects.
- **Interstitial:** Atom located in a “void” (I.e., a position that is not part of the lattice or basis) within the crystal structure.
- Frenkel Defect: A vacancy-interstitial pair.
- **Substitutional Impurity:** Impurity atoms (an atom that does not belong to the basis) that take up the lattice positions that are ordinarily occupied by the atoms that make up the crystal.
- **Interstitial Impurity:** Impurity atoms that are present in the interstitial sites.



# Point Defects



# Point Defects



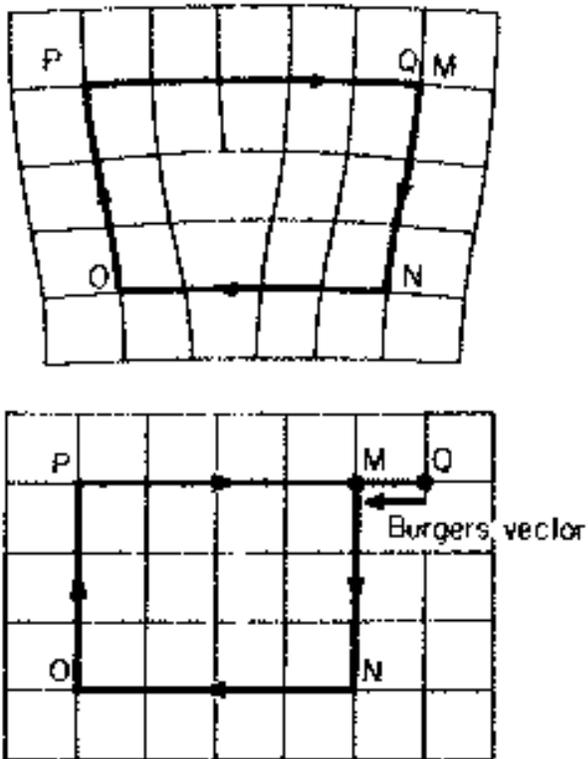
# Line Defects

- **Dislocations:** Boundary between two regions of a surface which are perfect themselves but are out of registry with each other. The resulting lattice distortion is centered along a line.
- **Burgers Vector,  $\mathbf{b}$ :** A vector by which the lattice on one side of an internal surface containing the dislocation line is displaced relative to the lattice on the other side.
- There are two special cases of dislocations
  - **Edge Dislocation:**  $\mathbf{b}$  and normal vector along the dislocation line  $\ell$  are perpendicular
  - **Screw Dislocation:**  $\mathbf{b}$  and normal vector along the dislocation line  $\ell$  are parallel



# Line Defects

## Edge Dislocation



## Screw Dislocation

