First Semester, 2018

Semiconductor Material Engineering

Jongwook Jeon

1.1.1 Composition

- Element semiconductor : Si, Ge

  Compound semiconductor : GaAs, ZnSe

  Alloy like : $Al_xGa_{1-x}As$

The x in alloy formulas is a fraction lying betw 0 and 1.

$Al_{0.3}Ga_{0.7}As$ → 3 Al and 7 Ga atoms per every 10 As atoms

1.1.2 Purity

- Extremely minute traces of impurity atoms called "dopants" can have a drastic effect on the electrical properties of semiconductors.

- Typically, dopant atoms at levels ranging from one per 10^8 to one impurity atom per 10^3 semiconductor atoms will be "purposely added" to the semiconductor to control its electrical properties.

1.1.3 Structure

- The spatial arrangement of atoms within a material plays an important role in determining the precise properties of the material.

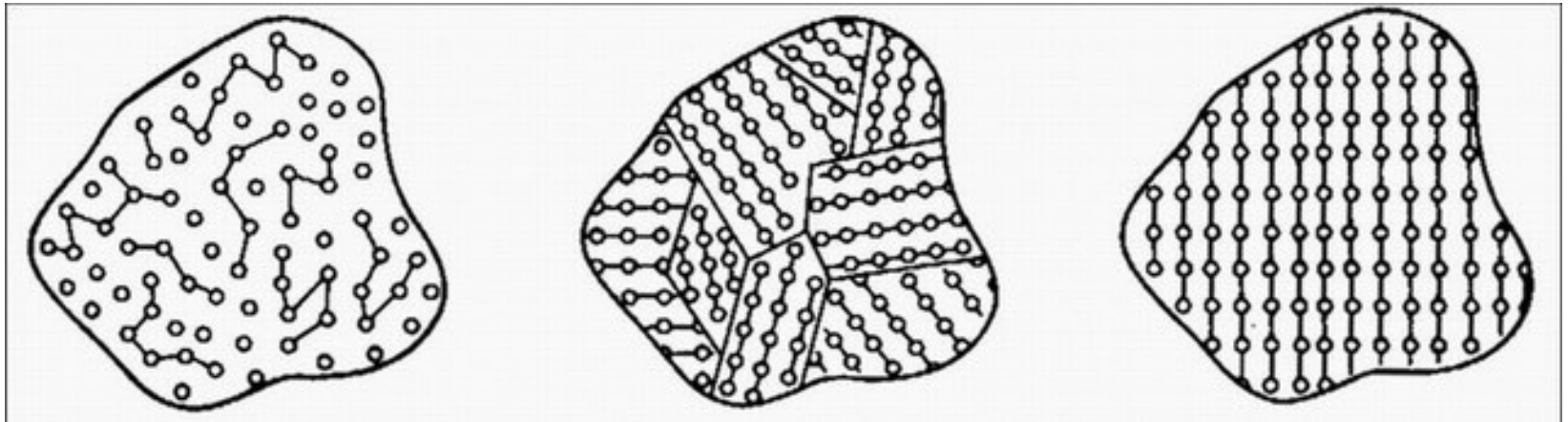


Figure 1.1 General classification of solids based on the degree of atomic order: (a) amorphous, (b) polycrystalline, and (c) crystalline.

1.1.3 Structure

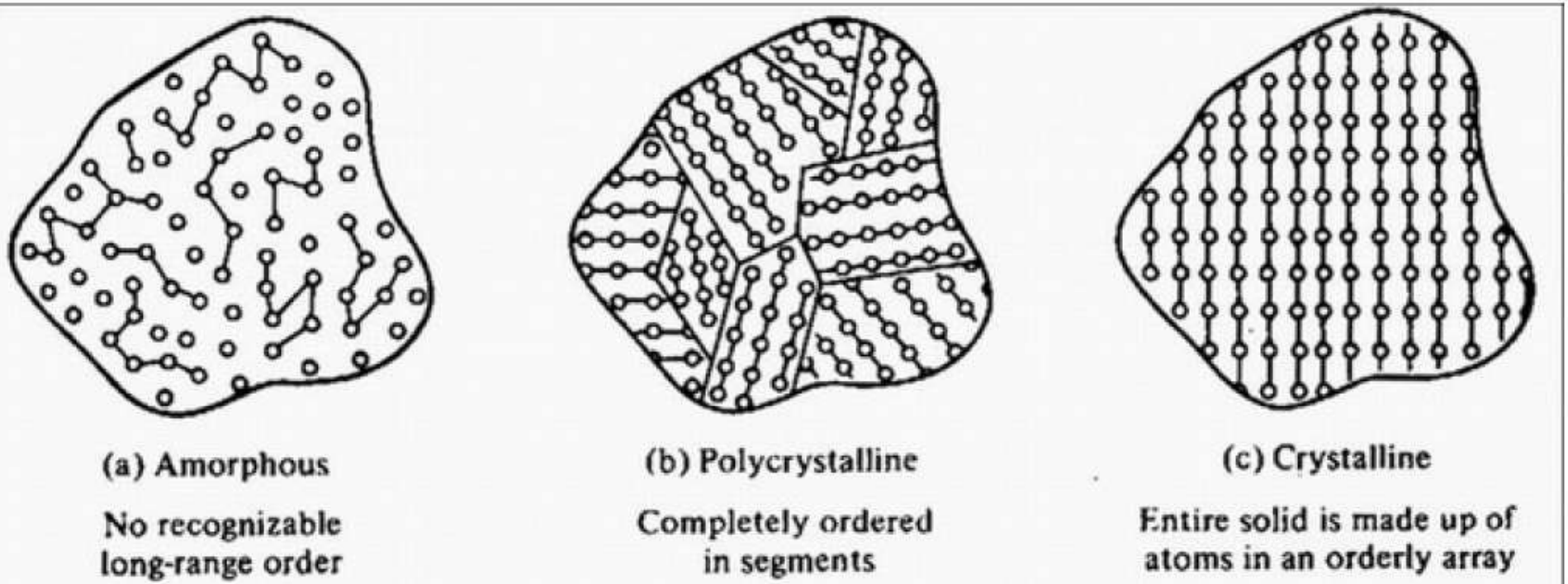


Figure 1.1 General classification of solids based on the degree of atomic order: (a) amorphous, (b) polycrystalline, and (c) crystalline.

: Amorphous Si TFT : switching element in LCD
Poly-Si : the gate of MOSFET, backplane of AMOLED
Crystalline Si : active region of MOSFET
Various devices employ Crystalline Si.

1.2 Crystal Structure

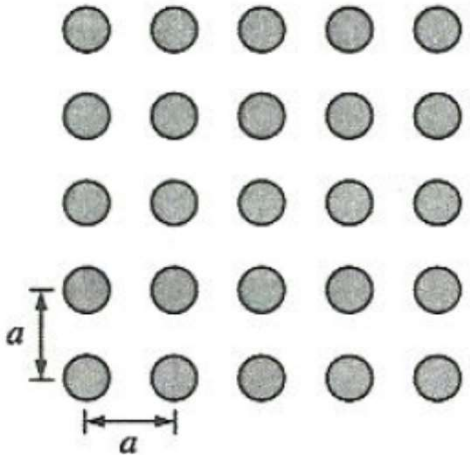
- **Additional information about the crystalline state**
- **More detailed picture of atomic arrangement of the crystalline structure**
  - Describing the spatial positioning of atoms
  - "Visualization" practice and Miller indices

Convenient shorthand notation identifying specific planes and directions

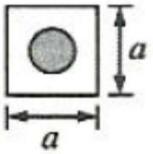
1.2.1 The Unit Cell Concept

- **"Unit" cell is a small portion of any given crystal which can reproduce the crystal**

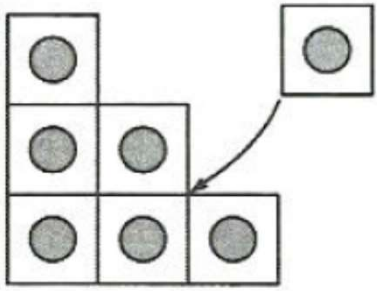
Unit cell describing atomic arrangement within crystal



2-D lattice

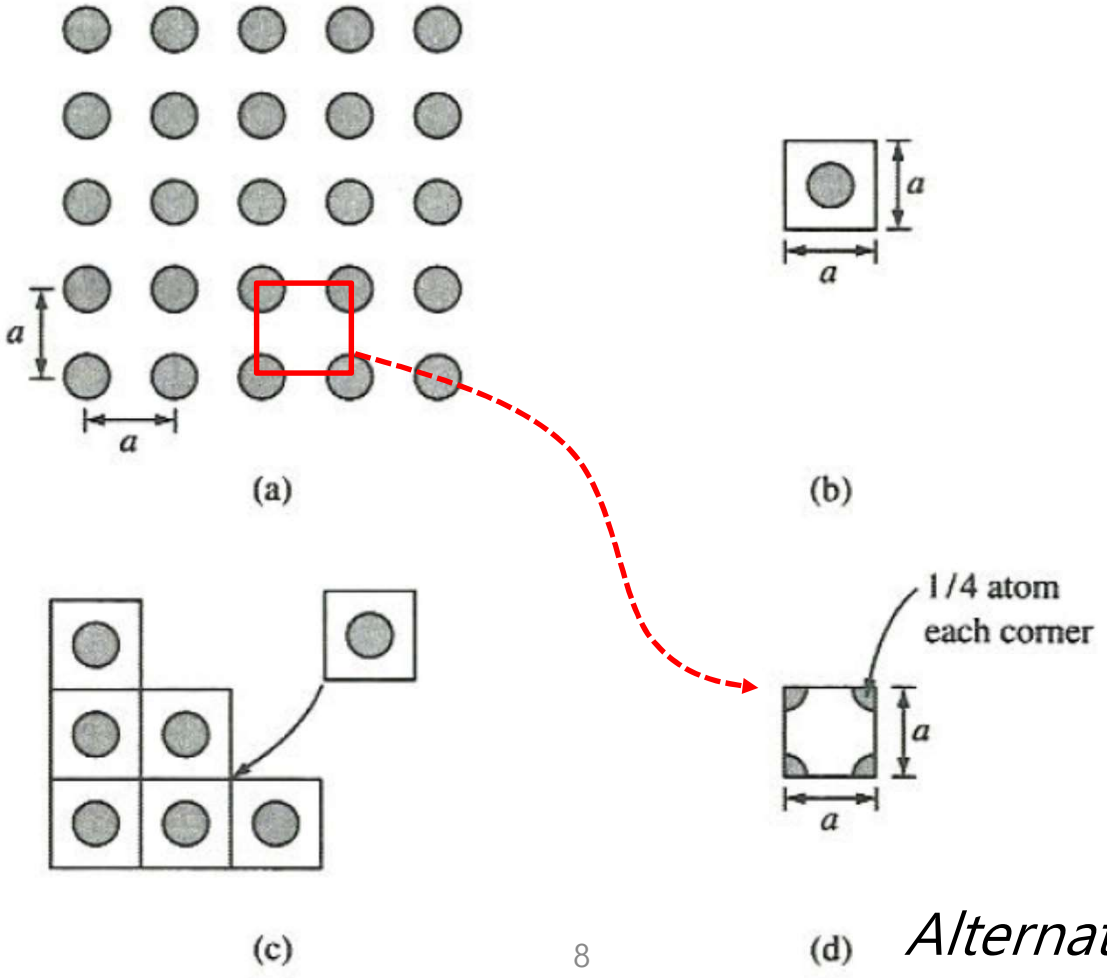


Unit cell



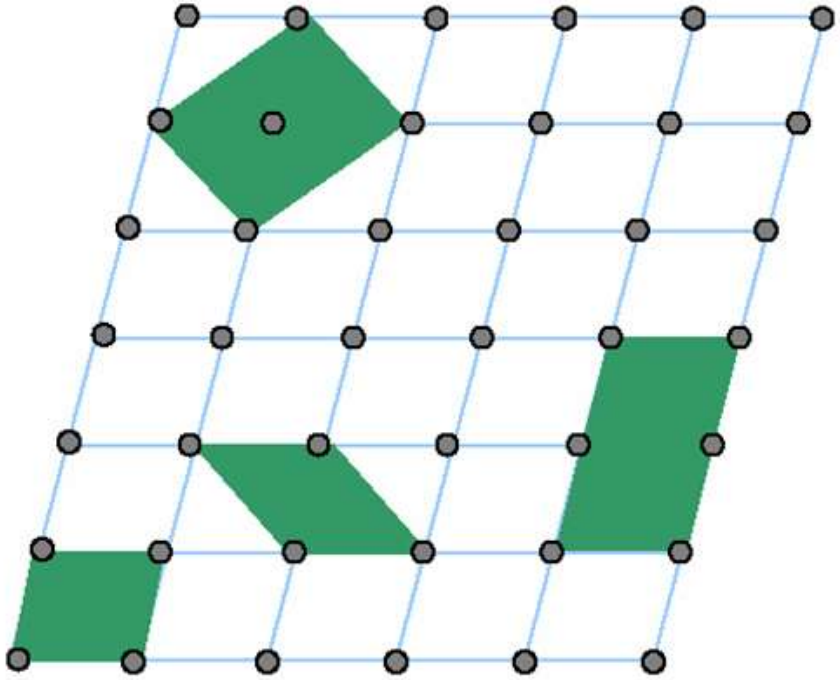
Reproduction

- **Some notifications**
  - **<u>Unit cells are not necessarily unique</u>**
  - Unit cell need not be primitive (smallest unit cell possible)



Alternative unit cell

- **Some notifications**
  - Unit cells are not necessarily unique
  - **Unit cell need not be primitive**

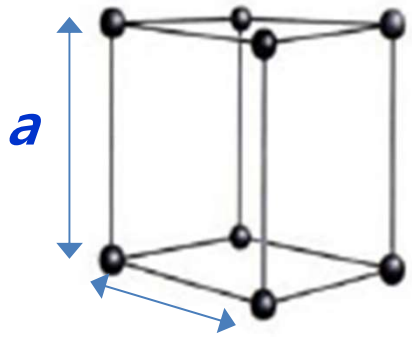


✓ Primitive cell?

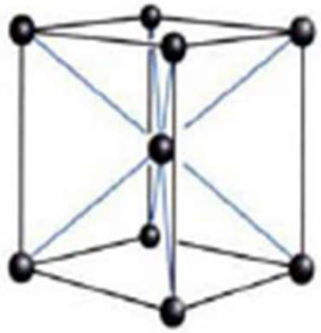
: smallest unit cell that can be repeated to form the lattice

Various unit cells examples

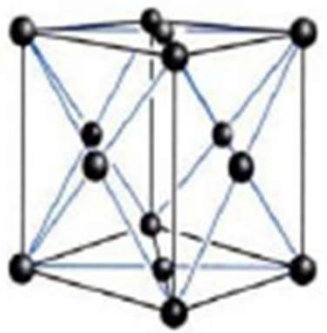
1.2.2 Simple 3-D unit cells



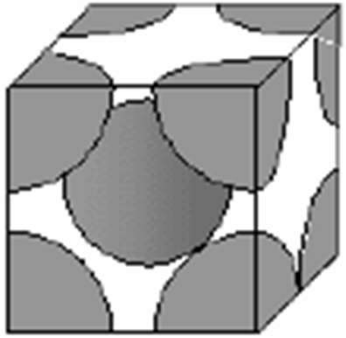
Cubic unit cell

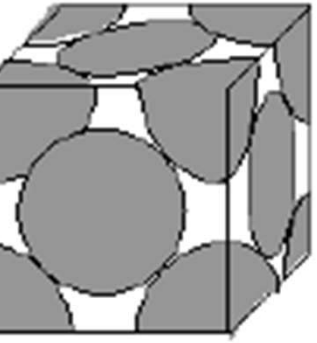


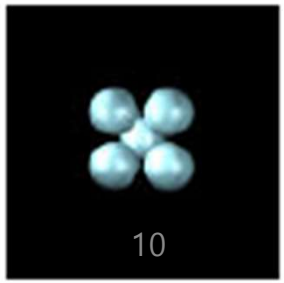
Body centered cubic unit cell

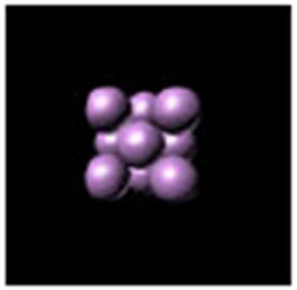


Face centered cubic unit cell

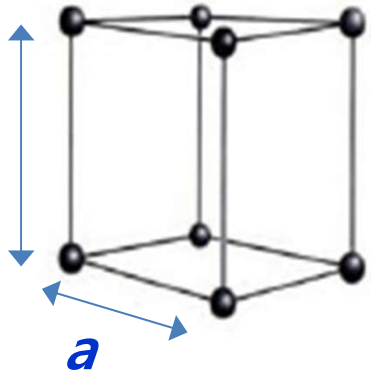


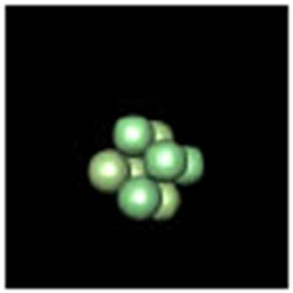






Simple Cubic unit cell





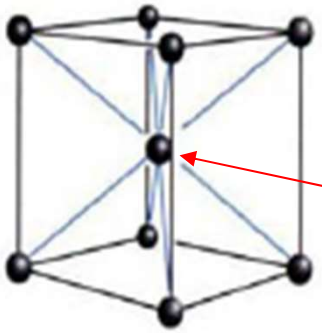
- **Cube with an atom positioned at each corner**

※ Lattice constant

: Planes of atoms parallel to the base plane are separated from one another by “lattice constant, a”

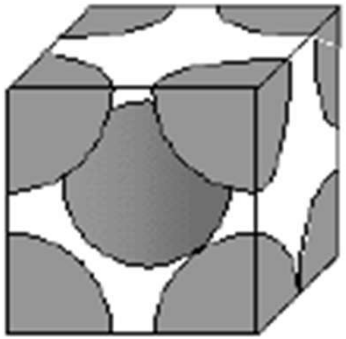
- **Simple cubic crystals are relatively rare, mostly because they tend to easily distort.**

Body Centered Cubic(BCC) unit cell



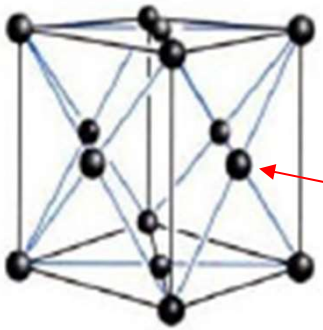
- Simple cubic cell

  + atom at the center of the cube



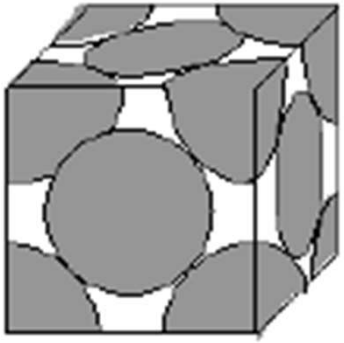
- lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten

Face Centered Cubic(FCC) unit cell

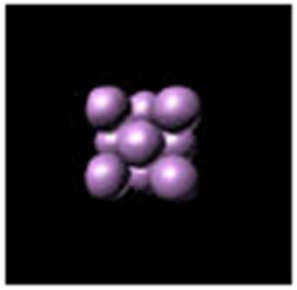


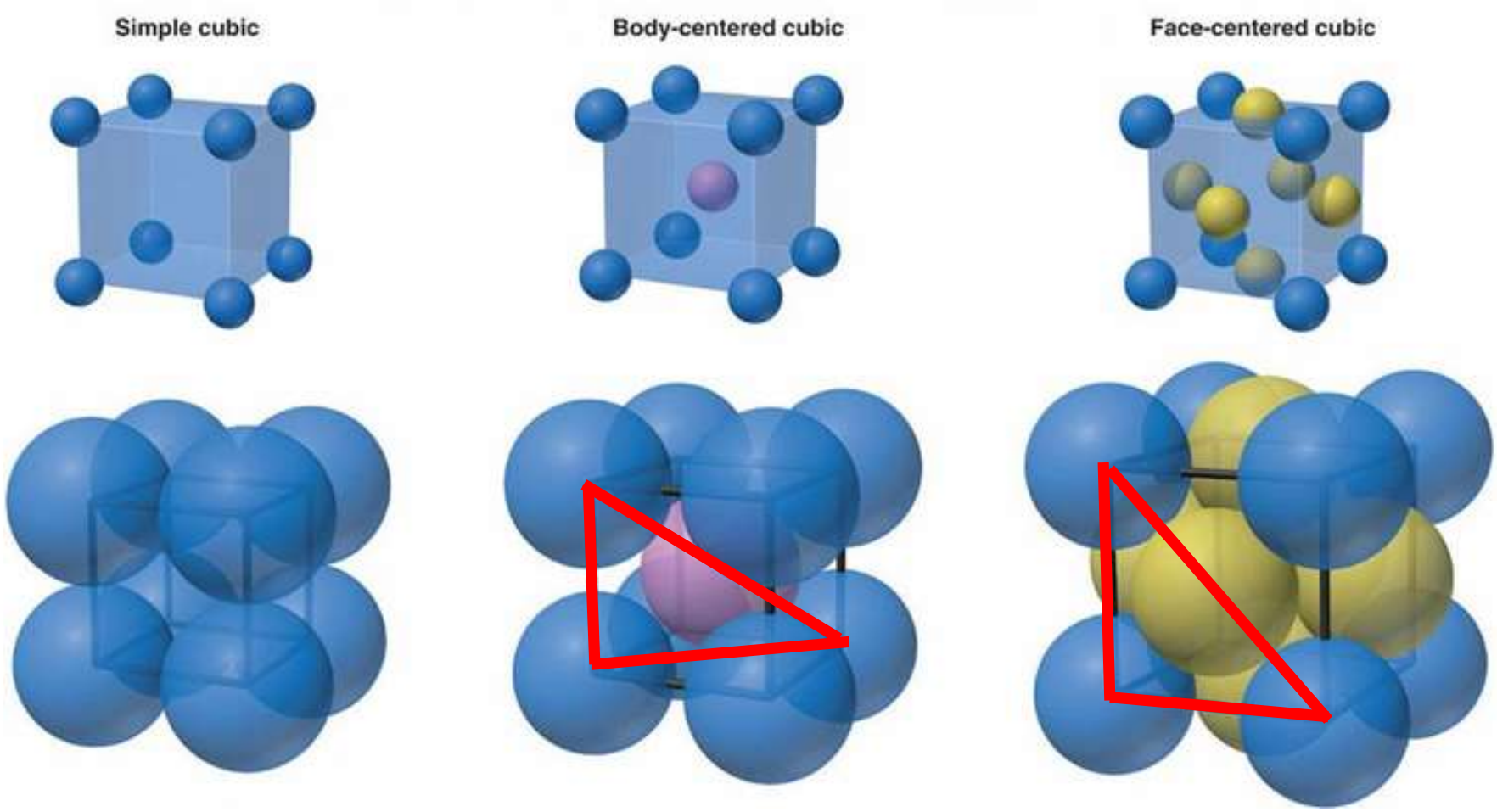
- Simple cubic cell

  + 6 atoms at each face of the cube



- aluminum, copper, gold, iridium, lead, nickel, platinum and silver





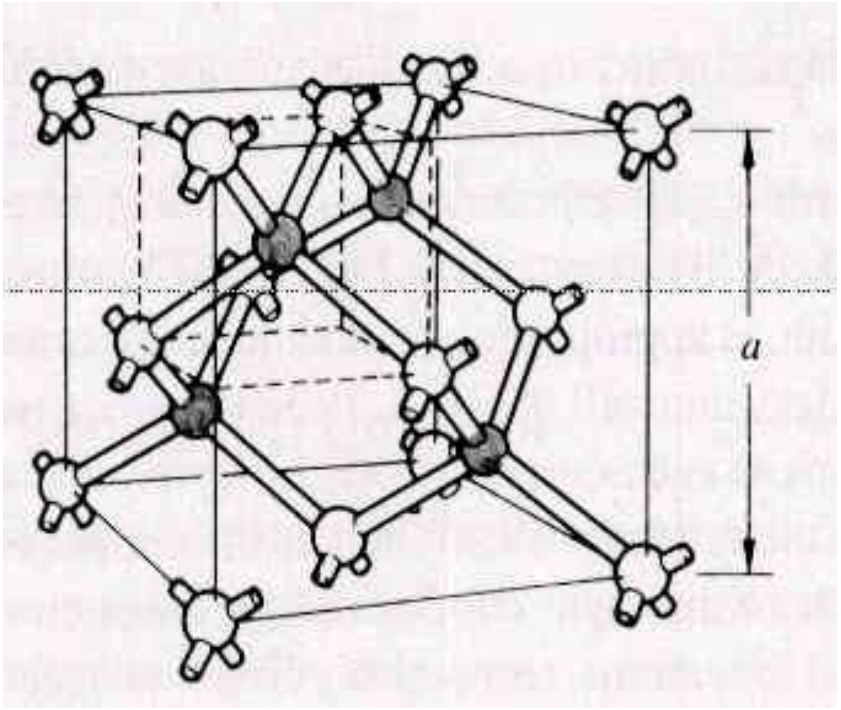
- **Whereas the simple cubic cell contains 1 atom, BCC and FCC cells contain 2 and 4 atoms, respectively.**

1.2.2 Simple 3-D unit cells

	sc	bcc	fcc
Volume/Cell	a^3	a^3	a^3
Atom/Cell	1	2	4
Atoms /Unit Volume	$1/a^3$	$2/a^3$	$4/a^3$
The # of nearest neighbors	6	8	12
The nearest neighbor distance	a	$\frac{\sqrt{3}}{2}a$	$\frac{\sqrt{2}}{2}a$

1.2.3 Semiconductor Lattices

- **In Si (and Ge), the lattice structure is described by the unit cell as below.**



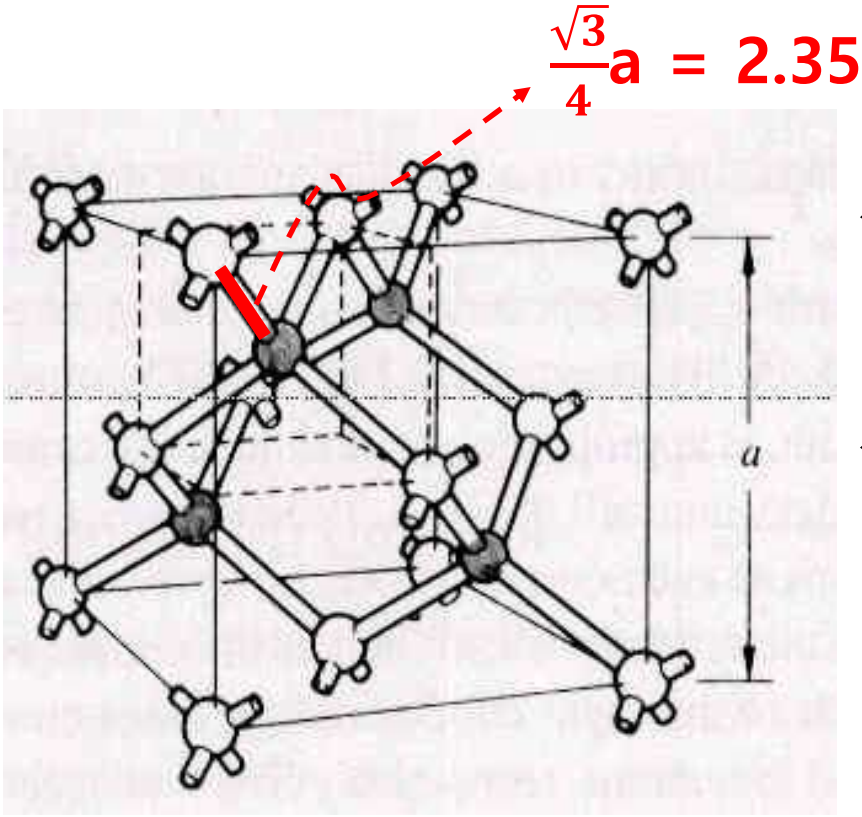
✓ **Diamond lattice structure**

It also characterizes diamond, a form of Col.IV element "carbon(C)"

✓ **Cubic with atoms at each corner and at each face of the cube similar to FCC + 4-additional atoms**

1.2.3 Semiconductor Lattices

- In Si (and Ge), the lattice structure is described by the unit cell as below.



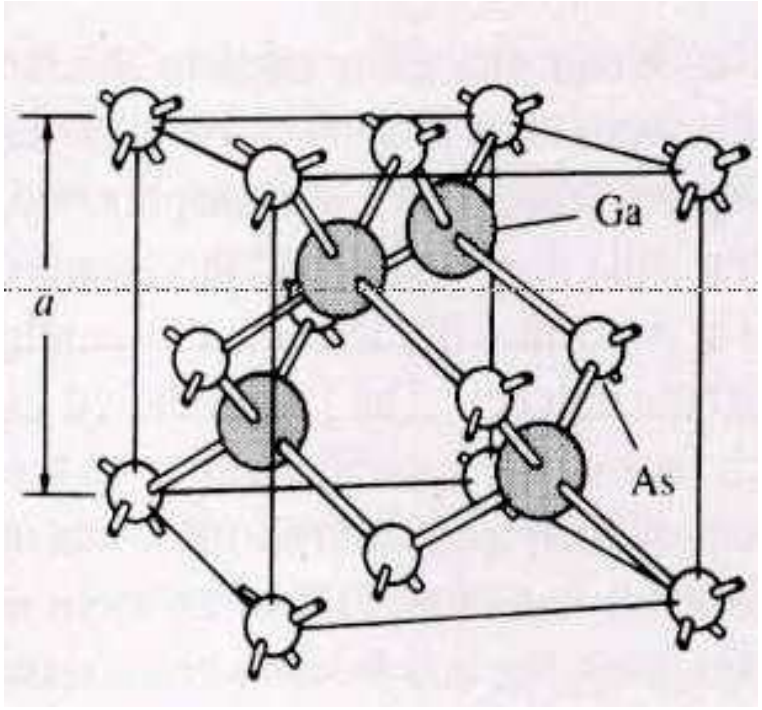
✓ a of Si @ RT = 5.43A

※ *1A = 10^{-8} cm*

✓ Total 8 atoms per Si unit cell → Si atom density is $8/a^3$, 5 x 10^{22} atoms/cm^3

1.2.3 Semiconductor Lattices

- **In GaAs, the lattice structure is described by the unit cell as below.**



✓ **<u>Zincblende</u> lattice structure**

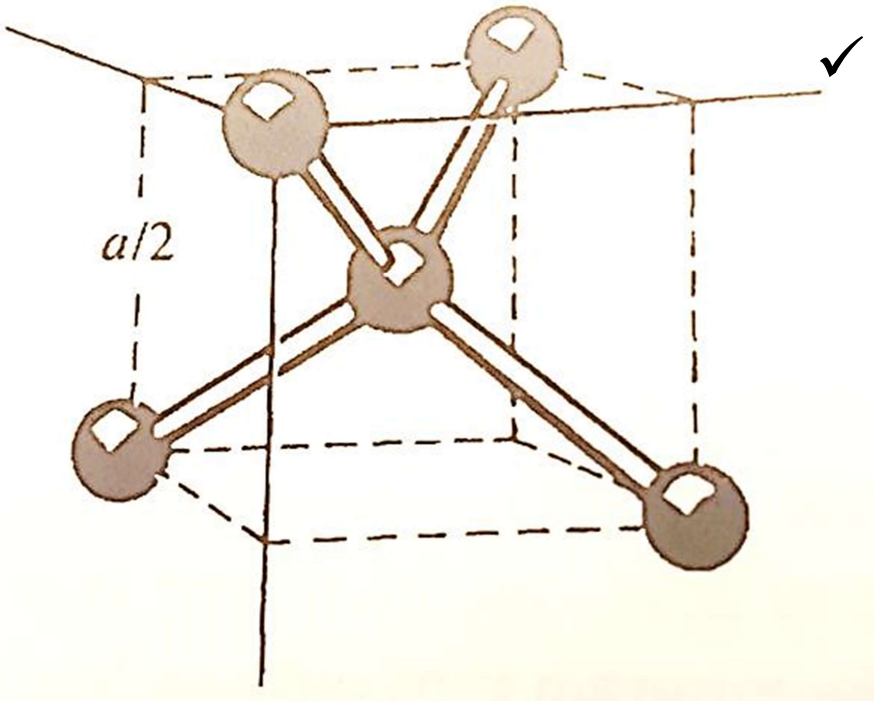
Most of III-V semic., has this str.

✓ Identical to the diamond lattice, except that lattice sites are apportioned equally betw Ga and As atoms.

✓ **a of GaAs @ RT = 5.65A**

1.2.3 Semiconductor Lattices

- **Atoms in the diamond and zincblende lattices have 4-nearest neighbors.**



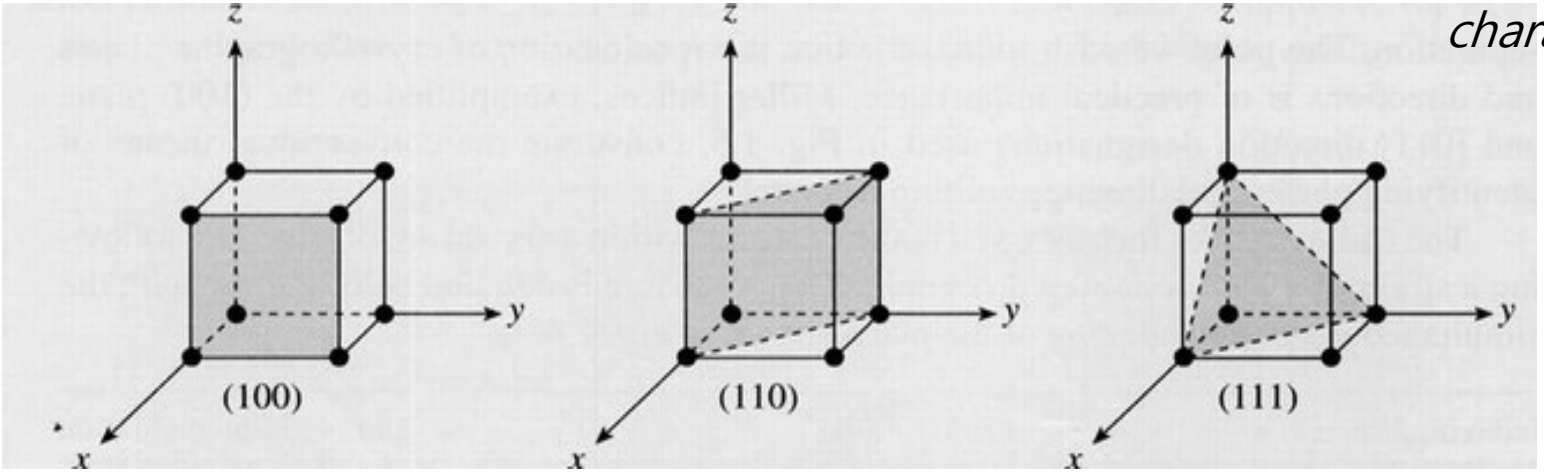
✓ **Chemical bonding within the major semiconductors is dominated by <u>the attraction betw any given atom and its four closest neighbors</u>**

1.2.4 Miller Indices

- **Single crystals of silicon used in device processing assumes the thin and round form → "Si-wafer"**

※ "Single" crystal(단결정) means atoms with orderly atom. Think about Poly-crystal(다결정) and Amorphous(비정질)

Different characteristics

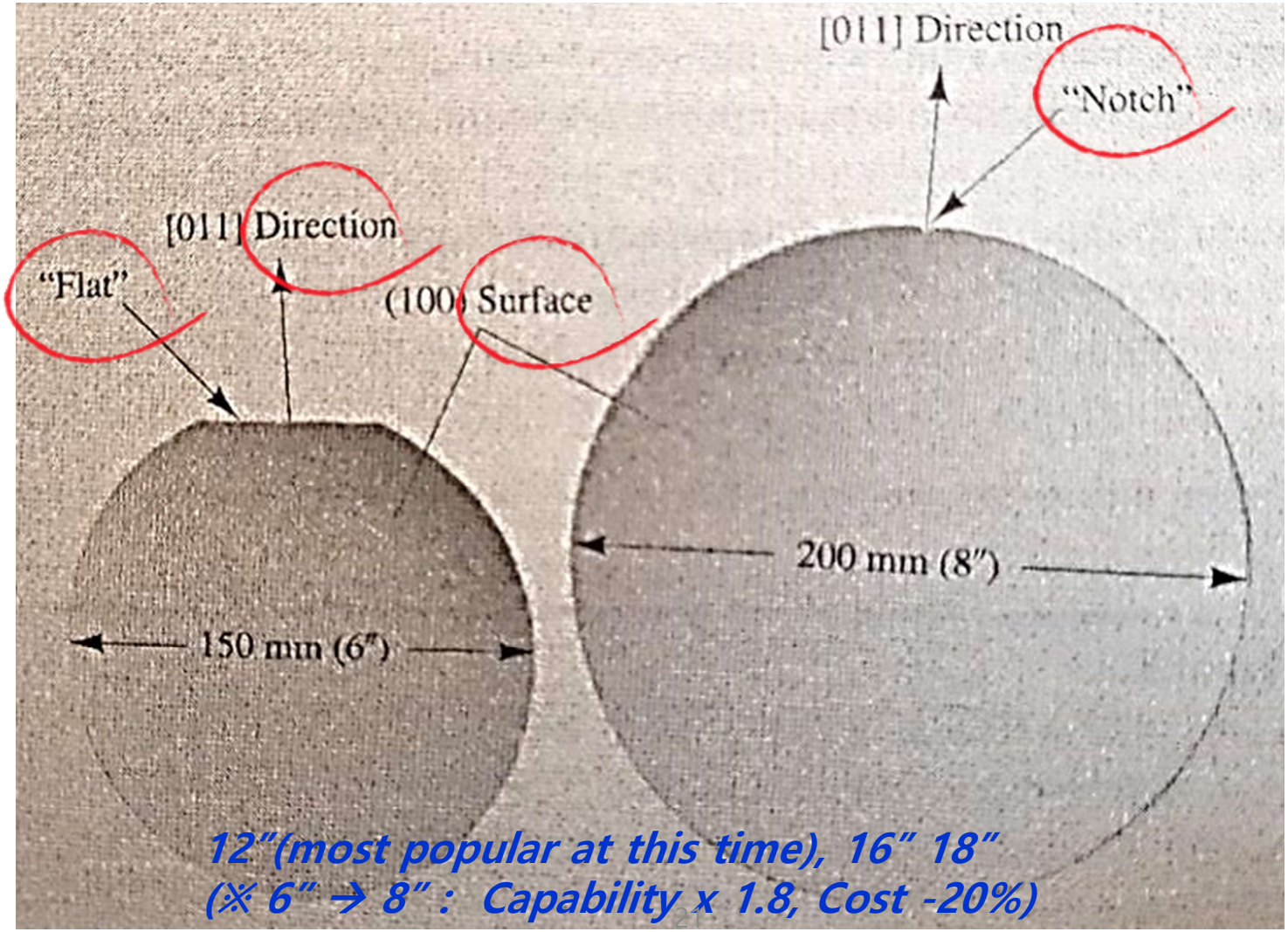


- **Wafer is carefully pre-oriented**
- **Using "Flat" or "Notch" to identify a reference direction**

1.2.4 Miller Indices

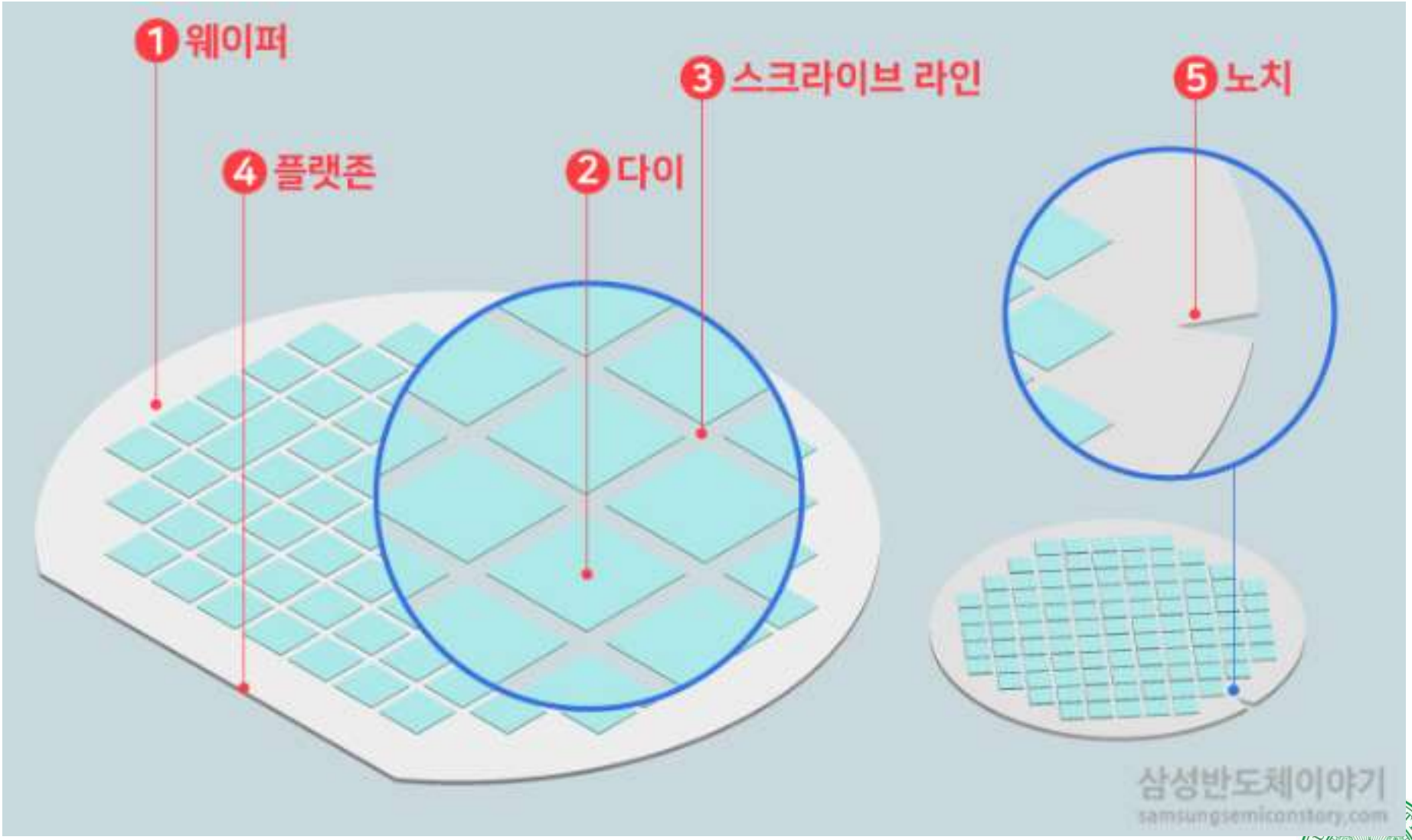
Convenient shorthand notation identifying specific planes and directions

- **Single crystal wafer**



12"(most popular at this time), 16" 18"
(※ 6" → 8" : Capability x 1.8, Cost -20%)

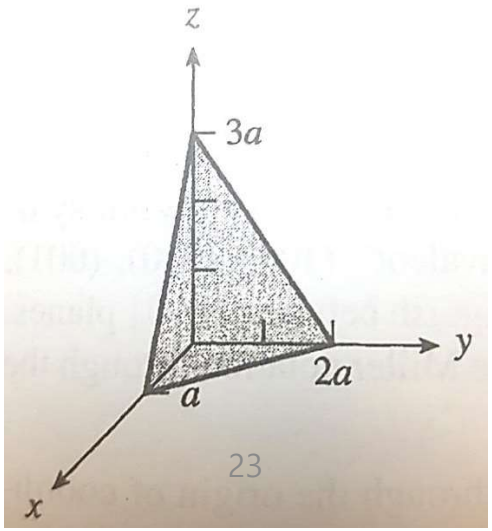
1.2.4 Miller Indices

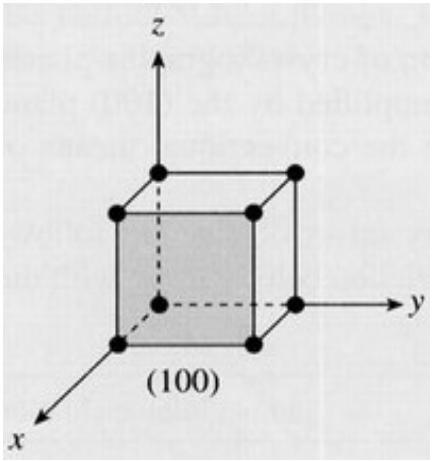


Notch technique can use more “die” than flat technique

● Miller indices are obtained by following 4-step procedure

Indexing Procedure	Sample Implementation
① After setting up coordinate axes along the edges of the unit cell, note where the plane to be indexed intercepts the axes. Divide each intercept value by the unit cell length along the respective coordinate axis. Record the resulting normalized (pure-number) intercept set in the order *x*, *y*, *z*.	1, 2, 3
② Invert the intercept values; that is, form [1/intercept]s.	1, ½, ⅓
③ Using an appropriate multiplier, convert the 1/intercept set to the smallest possible set of whole numbers.	6, 3, 2
④ Enclose the whole-number set in curvilinear brackets.	(632)



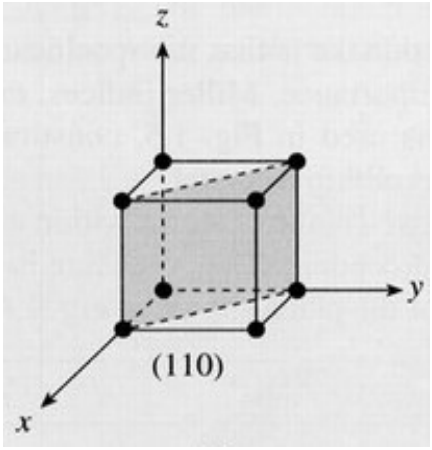


x, y, z → 1, ∞, ∞

1/1, 1/∞, 1/∞

1, 0, 0

(100)

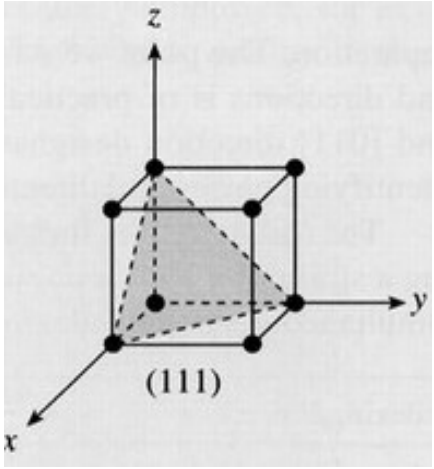


x, y, z → 1, 1, ∞

1/1, 1/1, 1/∞

1, 1, 0

(110)

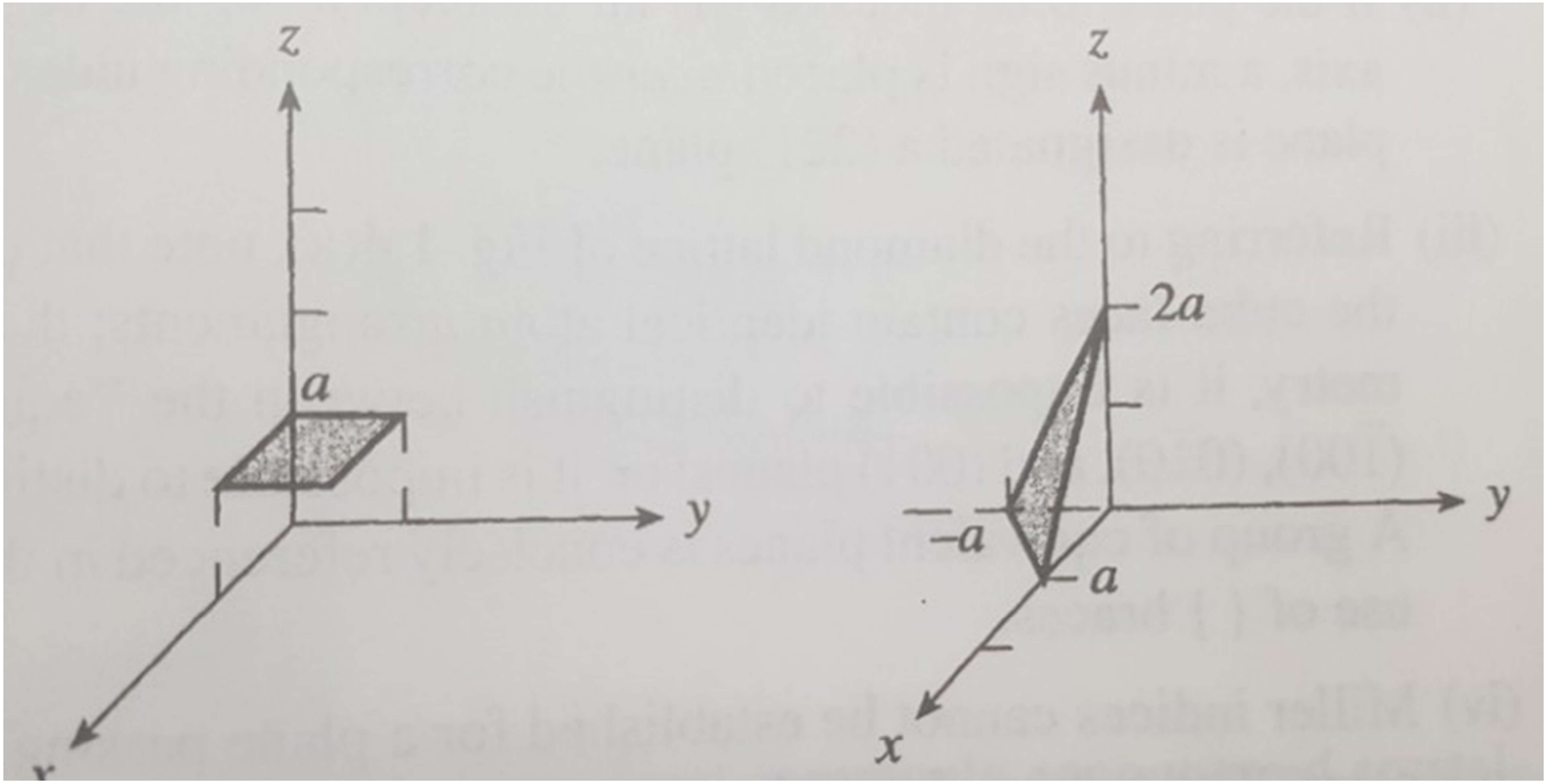


x, y, z → 1, 1, 1

1/1, 1/1, 1/1

1, 1, 1

(111)



x, y, z → ∞, ∞, 1

1/∞, 1/∞, 1/1

0, 0, 1

(001)

x, y, z → 1, -1, 2

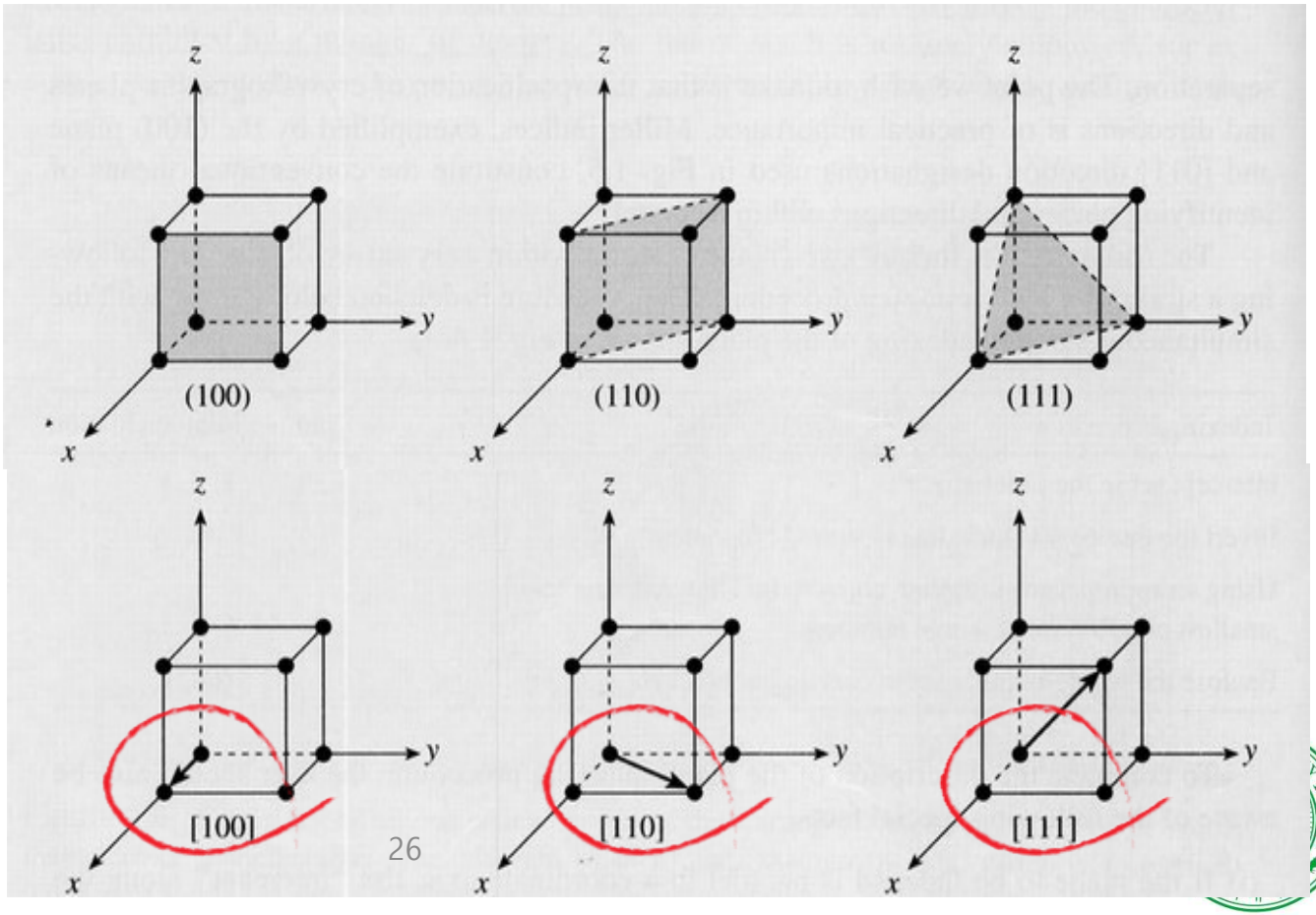
1/1, -1/1, 1/2

2, -2, 1

(2$\bar{2}$1)

- **A group of equivalent planes is concisely referenced in the Miller notation through the used of { } braces.**
  - → (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$ planes
  - → Because of crystal symmetry, it's impossible to distinguish each plane

- **<u>"Directions"</u>**



Exercise

P: For a cubic crystal lattice:

(a) Determine the Miller indices for the plane and direction vector shown in Fig. E1.4(a).

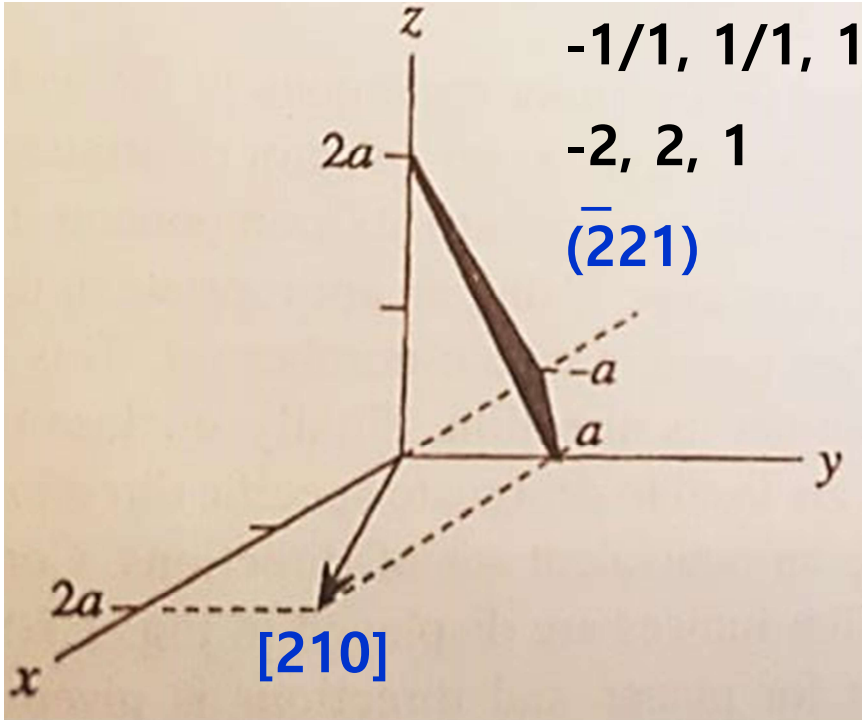
(b) Sketch the plane and direction vector characterized by (011) and [011], respectively.

x, y, z → -1, 1, 2

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

-2, 2, 1

$(\bar{2}21)$

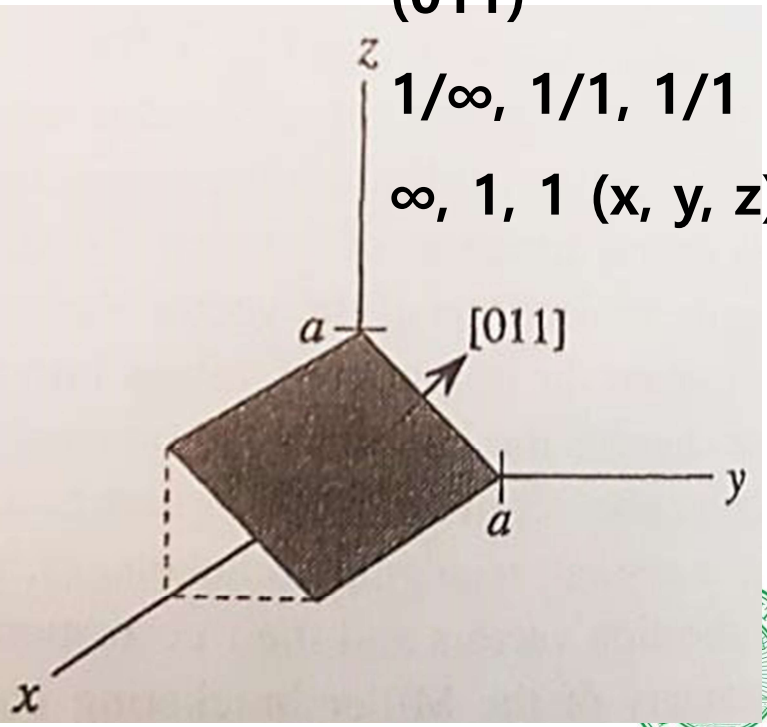


[210]

(011)

1/∞, 1/1, 1/1

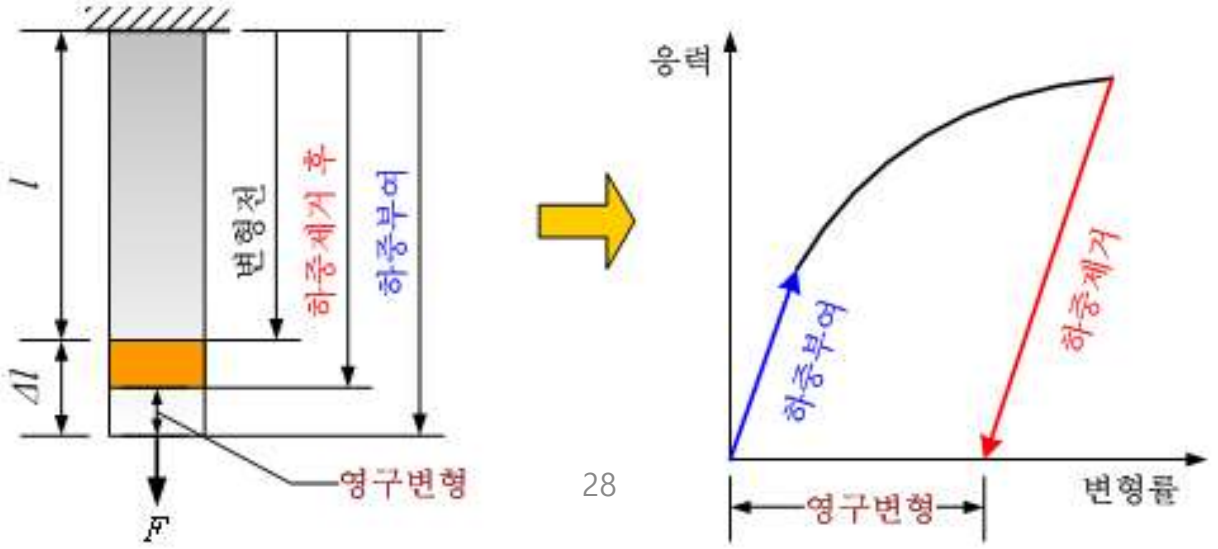
∞, 1, 1 (x, y, z)



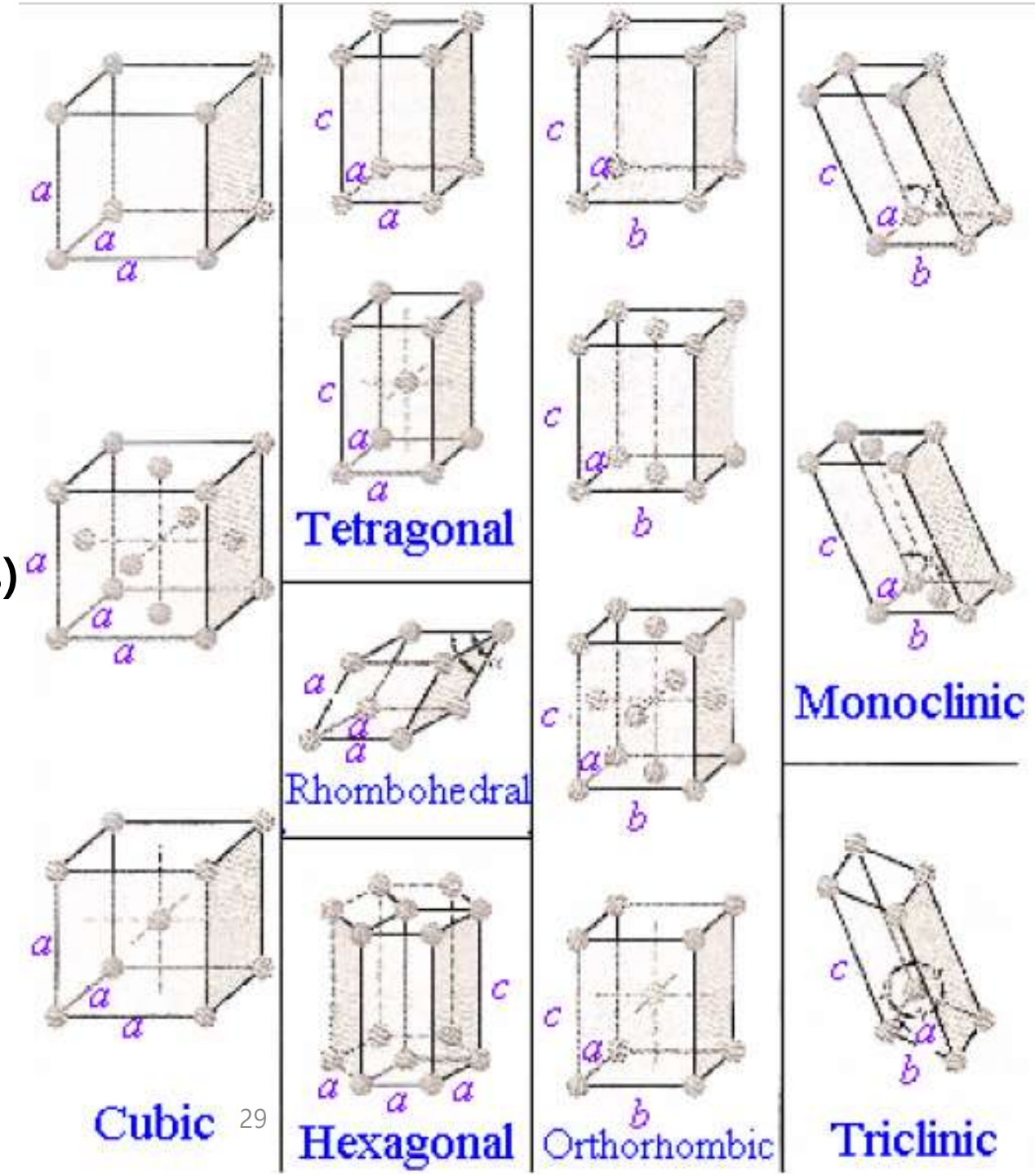
Advanced Physics – Crystal structure

- **In nature, 14 different types of crystal structure are found.**
- **Most metals (>90%) form BCC, FCC, or Hexagonal Close Packed (HCP) structures. (Simple cubic crystals are rare cases)**
  - Lattice structures with closely packed planes allow more plastic deformation than those that are not closely packed.

※ 탄성(Elasticity) : 외부 자극이 제거되면 물체를 원래 형상으로 복원하려는 성질
소성(Plasticity) : 외부 자극이 제거되어도 변형을 그대로 유지하려는 성질



- Only 7 different types of unit cells
- 14 standard (Bravais) unit cells could describe all possible lattice networks



- **Nearest neighbor distance : BCC (=$\sqrt{3}/2 \cdot a$), FCC (=$\sqrt{2}/2 \cdot a$)**

  → FCC will exhibit more ductility (deform more readily under load before breaking) than BCC
  유연성

  → BCC is not closely packed and forms strong metals than FCC

  → HCP lattices are closely packed, but not cubic. HCP metals like cobalt and zinc are not as ductile as FCC metals

- **Metals which have BCC structure are usually harder and less malleable than close-packed metals such as gold.**
  펴 늘릴 수 있는

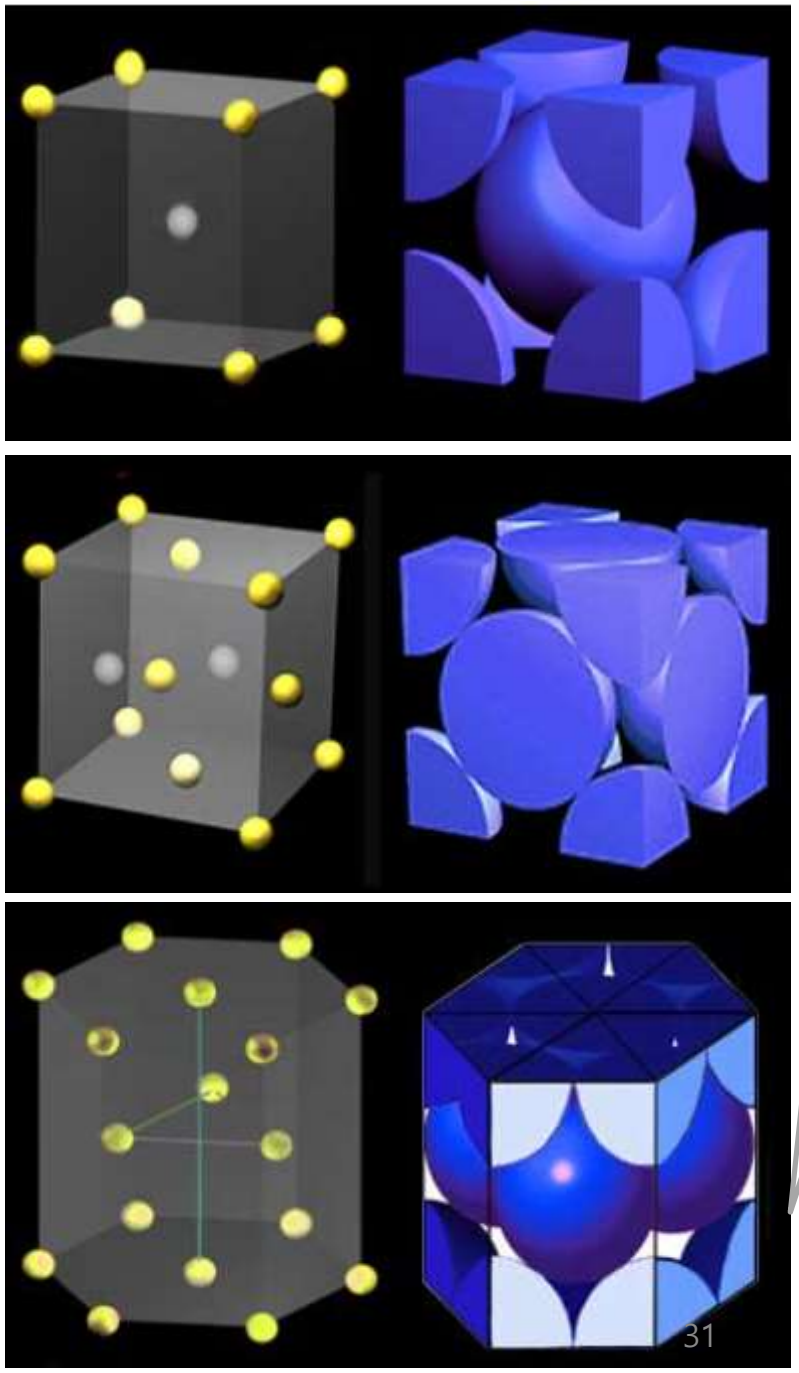
  → There are other important mechanisms for hardening materials, such as introducing impurities or defects

BCC

FCC

HCP

(not cubic)



6-atoms in HCP cell

beryllium, cadmium, magnesium, titanium, zinc and zirconium

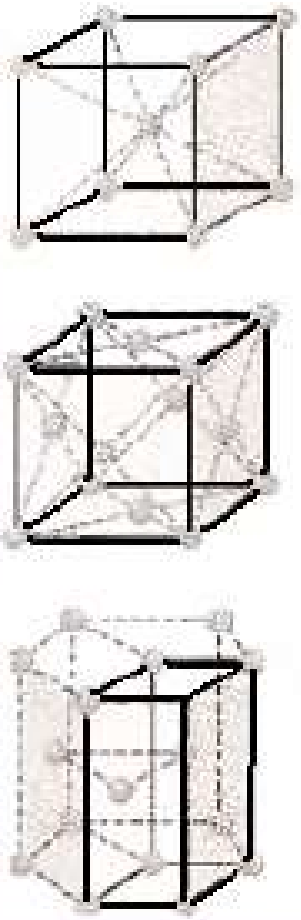
Cubic lattice structures allow slippage to occur more easily than non-cubic lattices, so hcp metals are not as ductile as the fcc metals.

- body-centered cubic (BCC)

	a (nm)	R (nm)
Cr	0.289	0.125
Fe	0.287	0.124
Mo	0.315	0.136
K	0.533	0.231
Na	0.429	0.186
Ta	0.330	0.143
W	0.316	0.137
V	0.304	0.132

- face-centered cubic (FCC)

	a (nm)	R (nm)
Al	0.405	0.143
Cu	0.3615	0.128
Au	0.408	0.144
Pb	0.495	0.175
Ni	0.352	0.125
Pt	0.393	0.139
Ag	0.409	0.144



- hexagonal close-packed (HCP)

	a	*c* (nm)	R (nm)
Al	0.2973	0.5618	0.143
Zn	0.2665	0.4947	0.133
Mg	0.3209	0.5209	0.160
Co	0.2507	0.4069	0.125
Zr	0.3231	0.5148	0.160
Ti	0.2950	0.4683	0.147
Be	0.2286	0.3584	0.113

- **The structure can change depending on temperature.**

metal	crystal structure at room temperature	at other temperature
Ca	FCC	BCC (> 447°C)
Co	HCP	FCC (> 427°C)
Hf	HCP	BCC (> 1742°C)
Fe	BCC (α)	FCC (912-1394°C) (γ)
		BCC (> 1394°C) (δ)
Li	BCC	HCP (< -193°C)
Na	BCC	HCP (< -233°C)
Tl	HCP	BCC (> 234°C)
Ti	HCP	BCC (> 883°C)
Y	HCP	BCC (> 1481°C)
Zr	HCP	BCC (> 872°C)