第一章

1.1 Semiconductor Materials

1.2 Types of Solids

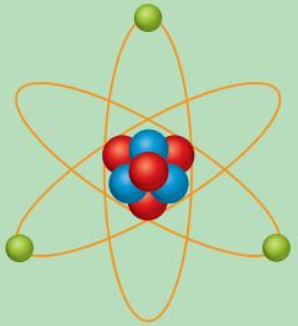
1.3 Space Lattices

1.4 The Diamond Structure

1.5 Atomic Bonding

原子結構

原子



原子核

- 直徑約 $10^{-14} \sim 10^{-15}$ m

核外：電子

- 帶 1.602×10^{-19} 庫侖的**負電**
- 質量約 9.11×10^{-31} kg

中子

- **不帶電**
- 質量為 1.675×10^{-27} kg 約和質子相同
- **決定同位素之存在**

質子

- 帶 1.602×10^{-19} 庫侖的**正電**
- 平均質量約 1.673×10^{-27} kg，約電子的 1836 倍
- **決定元素之種類**與在週期表的位置

氫原子模型

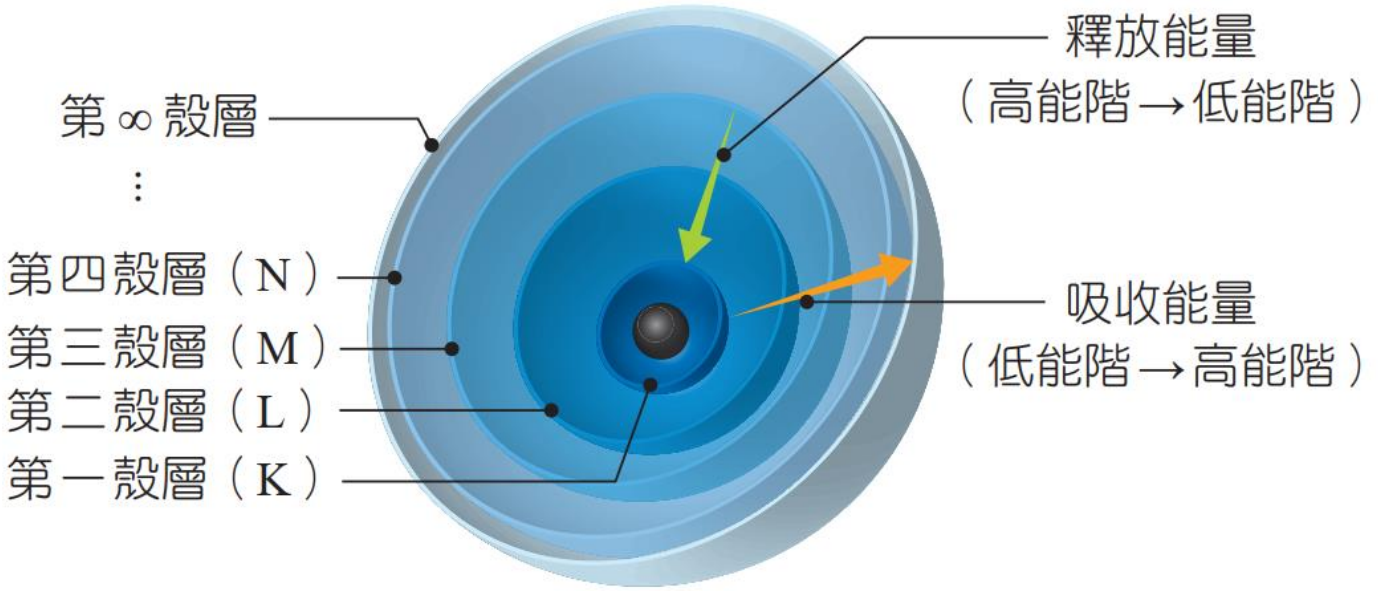


圖 1-32　原子中同心球切面，電子在不同能階間的躍遷示意圖

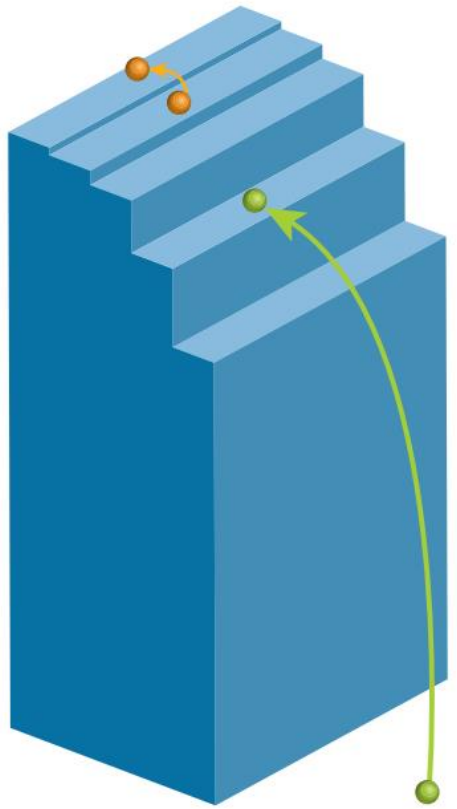
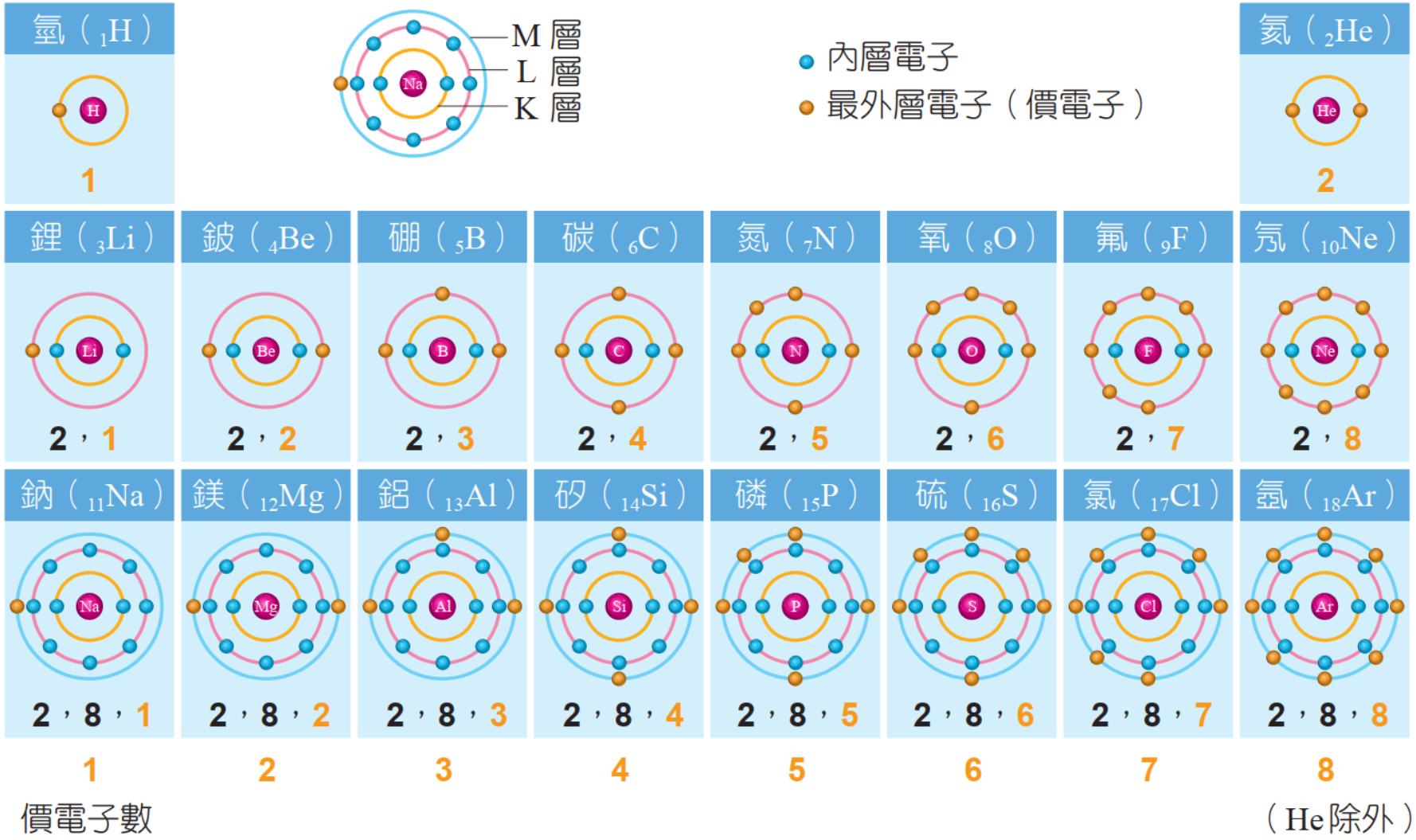


圖 1-31　電子能階示意圖

電子排列示意圖


氫（$_1$H）
H
1
M 層
L 層
K 層
Na
內層電子
最外層電子（價電子）
氦（$_2$He）
He
2
鋰（$_3$Li）
Li
2，1
鈹（$_4$Be）
Be
2，2
硼（$_5$B）
B
2，3
碳（$_6$C）
C
2，4
氮（$_7$N）
N
2，5
氧（$_8$O）
O
2，6
氟（$_9$F）
F
2，7
氖（$_{10}$Ne）
Ne
2，8
鈉（$_{11}$Na）
Na
2，8，1
鎂（$_{12}$Mg）
Mg
2，8，2
鋁（$_{13}$Al）
Al
2，8，3
矽（$_{14}$Si）
Si
2，8，4
磷（$_{15}$P）
P
2，8，5
硫（$_{16}$S）
S
2，8，6
氯（$_{17}$Cl）
Cl
2，8，7
氬（$_{18}$Ar）
Ar
2，8，8
1
2
3
4
5
6
7
8
價電子數
（He除外）

半導體材料

半導體，也就是導電性質介於金屬與絕緣體中間

- 元素半導體 elemental semiconductor，如 Si, Ge
- 化合物半導體 compound semiconductor，如 GaAs, InP

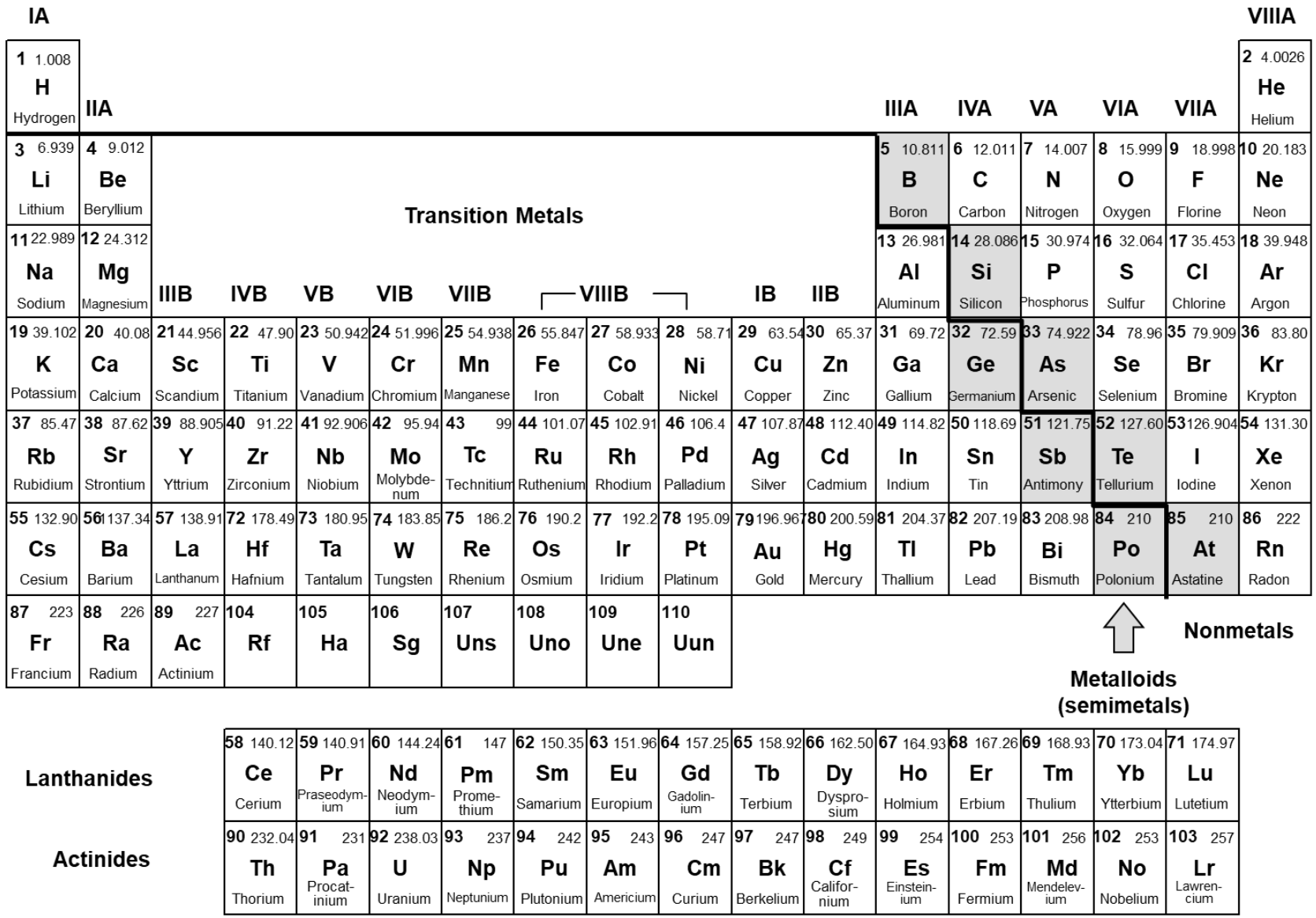
Table 1.1 | A portion of the periodic table

III	IV	V
5 **B** Boron	6 **C** Carbon	
13 **Al** Aluminum	14 **Si** Silicon	15 **P** Phosphorus
31 **Ga** Gallium	32 **Ge** Germanium	33 **As** Arsenic
49 **In** Indium		51 **Sb** Antimony

Table 1.2 | A list of some semiconductor materials

Elemental semiconductors	
Si	Silicon
Ge	Germanium
Compound semiconductors	
AlP	Aluminum phosphide
AlAs	Aluminum arsenide
GaP	Gallium phosphide
GaAs	Gallium arsenide
InP	Indium phosphide

週期表


IA
VIIIA
1 1.008 H Hydrogen
IIA
2 4.0026 He Helium
IIIA
IVA
VA
VIA
VIIA
3 6.939 Li Lithium
4 9.012 Be Beryllium
Transition Metals
5 10.811 B Boron
6 12.011 C Carbon
7 14.007 N Nitrogen
8 15.999 O Oxygen
9 18.998 F Florine
10 20.183 Ne Neon
11 22.989 Na Sodium
12 24.312 Mg Magnesium
IIIB
IVB
VB
VIB
VIIB
VIIIB
IB
IIB
13 26.981 Al Aluminum
14 28.086 Si Silicon
15 30.974 P Phosphorus
16 32.064 S Sulfur
17 35.453 Cl Chlorine
18 39.948 Ar Argon
19 39.102 K Potassium
20 40.08 Ca Calcium
21 44.956 Sc Scandium
22 47.90 Ti Titanium
23 50.942 V Vanadium
24 51.996 Cr Chromium
25 54.938 Mn Manganese
26 55.847 Fe Iron
27 58.933 Co Cobalt
28 58.71 Ni Nickel
29 63.54 Cu Copper
30 65.37 Zn Zinc
31 69.72 Ga Gallium
32 72.59 Ge Germanium
33 74.922 As Arsenic
34 78.96 Se Selenium
35 79.909 Br Bromine
36 83.80 Kr Krypton
37 85.47 Rb Rubidium
38 87.62 Sr Strontium
39 88.905 Y Yttrium
40 91.22 Zr Zirconium
41 92.906 Nb Niobium
42 95.94 Mo Molybde-num
43 99 Tc Technitium
44 101.07 Ru Ruthenium
45 102.91 Rh Rhodium
46 106.4 Pd Palladium
47 107.87 Ag Silver
48 112.40 Cd Cadmium
49 114.82 In Indium
50 118.69 Sn Tin
51 121.75 Sb Antimony
52 127.60 Te Tellurium
53 126.904 I Iodine
54 131.30 Xe Xenon
55 132.90 Cs Cesium
56 137.34 Ba Barium
57 138.91 La Lanthanum
72 178.49 Hf Hafnium
73 180.95 Ta Tantalum
74 183.85 W Tungsten
75 186.2 Re Rhenium
76 190.2 Os Osmium
77 192.2 Ir Iridium
78 195.09 Pt Platinum
79 196.967 Au Gold
80 200.59 Hg Mercury
81 204.37 Tl Thallium
82 207.19 Pb Lead
83 208.98 Bi Bismuth
84 210 Po Polonium
85 210 At Astatine
86 222 Rn Radon
87 223 Fr Francium
88 226 Ra Radium
89 227 Ac Actinium
104 Rf
105 Ha
106 Sg
107 Uns
108 Uno
109 Une
110 Uun
Nonmetals
Metalloids (semimetals)
Lanthanides
58 140.12 Ce Cerium
59 140.91 Pr Praseodym-ium
60 144.24 Nd Neodym-ium
61 147 Pm Prome-thium
62 150.35 Sm Samarium
63 151.96 Eu Europium
64 157.25 Gd Gadolin-ium
65 158.92 Tb Terbium
66 162.50 Dy Dyspro-sium
67 164.93 Ho Holmium
68 167.26 Er Erbium
69 168.93 Tm Thulium
70 173.04 Yb Ytterbium
71 174.97 Lu Lutetium
Actinides
90 232.04 Th Thorium
91 231 Pa Procat-inium
92 238.03 U Uranium
93 237 Np Neptunium
94 242 Pu Plutonium
95 243 Am Americium
96 247 Cm Curium
97 247 Bk Berkelium
98 249 Cf Califor-nium
99 254 Es Einstein-ium
100 253 Fm Fermium
101 256 Md Mendelev-ium
102 253 No Nobelium
103 257 Lr Lawren-cium

固態物質種類

非晶 Amorphous

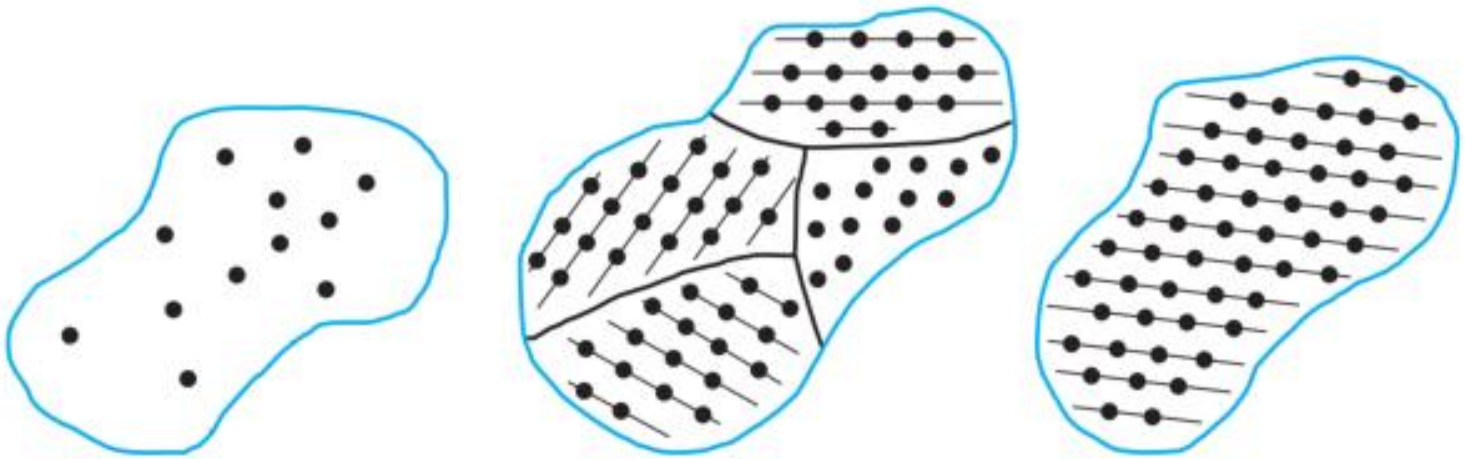
有序程度非常低 (degree of order)，原子排列雜亂無章 (< 10 nm)

多晶 Poly-crystalline

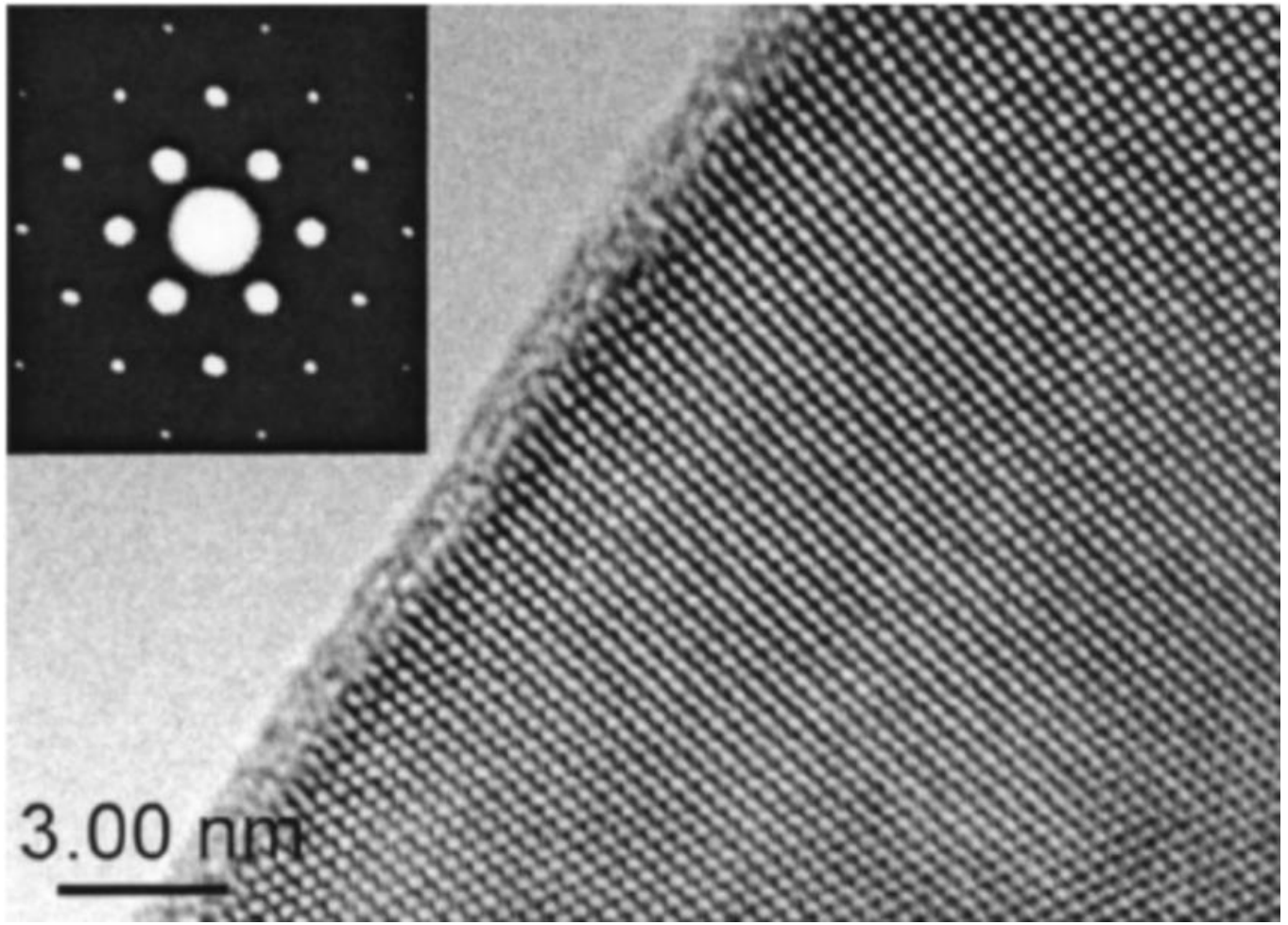
有序程度中等 (100 nm - 10 μm)，每個有序排列的區域稱為晶粒 (grains)，每個晶粒之間的大小與排列方向不盡相同。

單晶 Single-crystalline

材料內原子的排序程度非常高，方向一致，幾乎呈現完美狀態



單晶矽



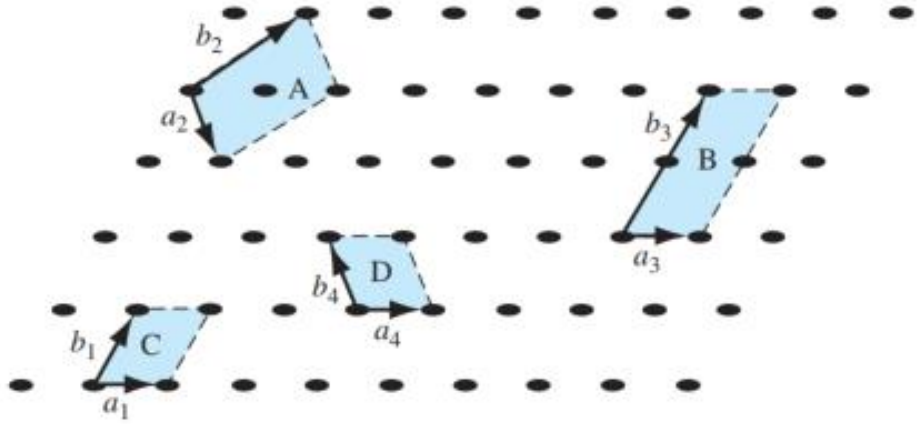
Space Lattices

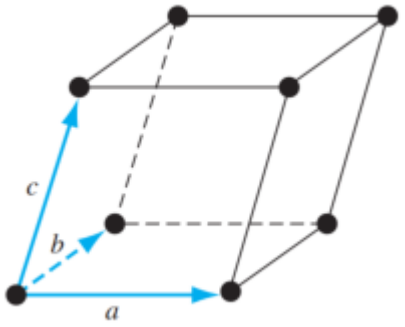
晶格 (Lattice)：一個區域或空間中，具有規則幾何排列的點或物體

單位晶胞 (Unit cell)：具對稱性的原子排列，可在空間上重複構建整個晶格

晶格常數 (Lattice constant)：單位晶胞的物理尺寸，通常以向量描述

原胞 (Primitive cell)：無法再被切割的單位晶格



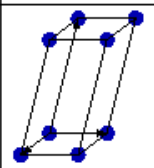
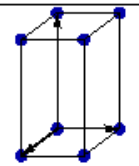
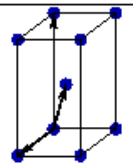
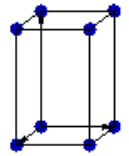
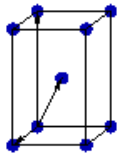
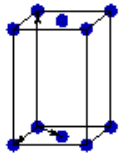
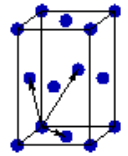
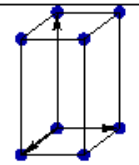
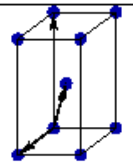
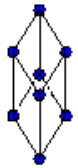
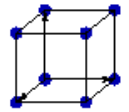
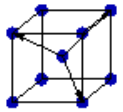
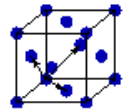
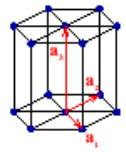


$$\vec{r} = p\vec{a} + q\vec{b} + s\vec{c}$$

Primitive vector

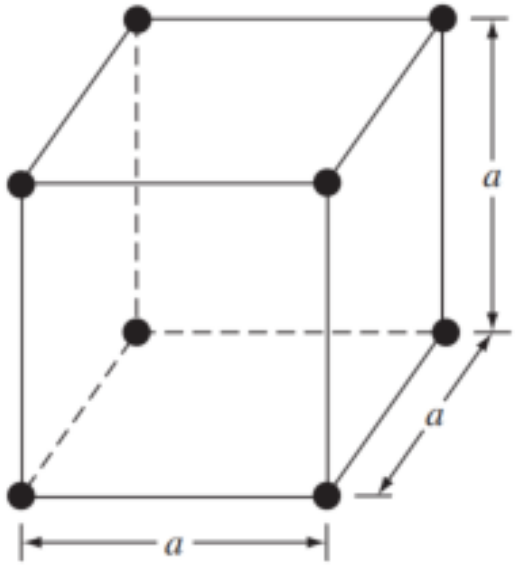
p, q, s: integer

Crystal System

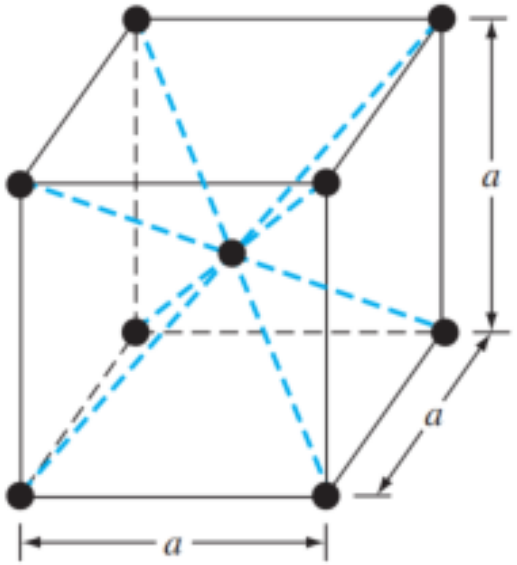
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
三斜晶系 Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
單斜晶系 Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
正交晶系 Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
四方晶系 Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
菱方晶系 Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
立方晶系 Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
六方晶系 Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Cubic crystal system

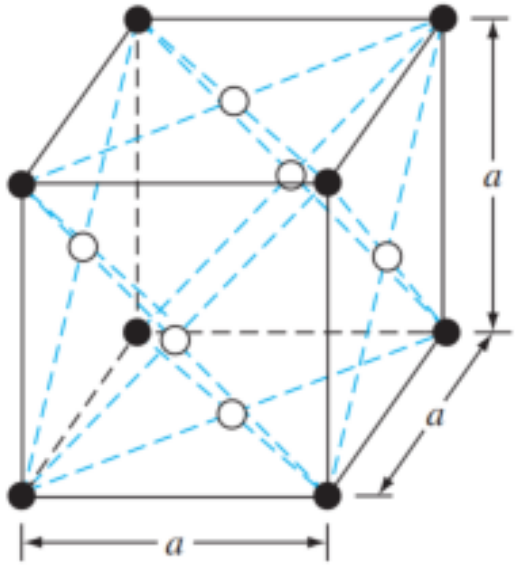
Simple cubic
(SC)
簡單立方



Body-centered cubic
(BCC)
體心立方



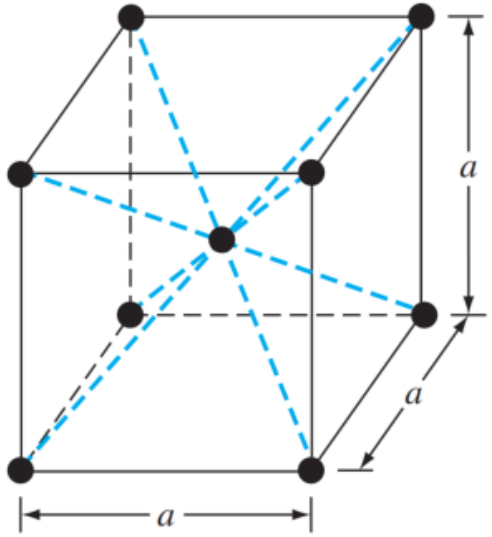
Face-centered cubic
(FCC)
面心立方



Example 1.1 Find the Volume Density

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 $a = 5\ \text{Å} = 5 \times 10^{-8}$ 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.

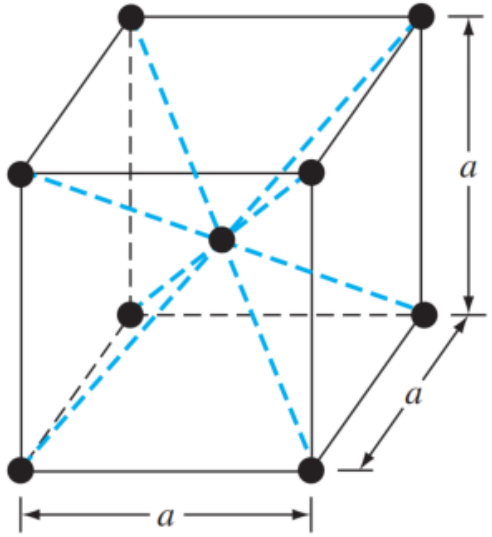


$$\text{Volume Density} = \frac{\#\ atoms\ per\ unit\ cell}{volume\ of\ unit\ cell}$$

Example 1.1 Find the Volume Density

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

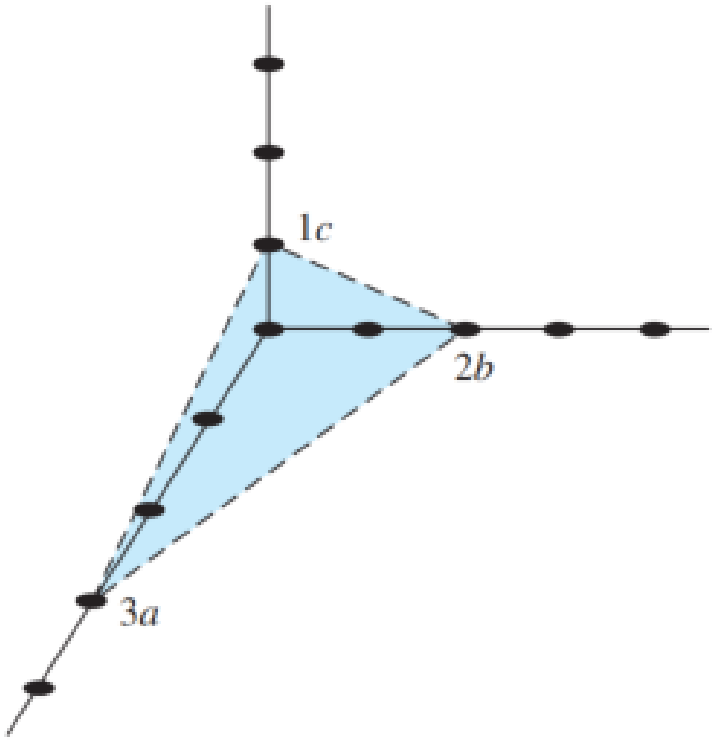
Consider a single-crystal material that is a body-centered cubic, as shown in Figure 1.5b, with a lattice constant $a = 5\ \text{Å} = 5 \times 10^{-8}$ cm. A corner atom is shared by eight unit cells that meet at each corner so that each corner atom effectively contributes one-eighth of its volume to 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.



$$\frac{\left(8\times\frac{1}{8}+1\right)}{\left(5\times10^{-8}\right)^3}=1.6\times10^{22} \quad \text{Atoms/cm}^3$$

Crystal Planes and Miller Indices

如何描述一個晶面 → Miller indices

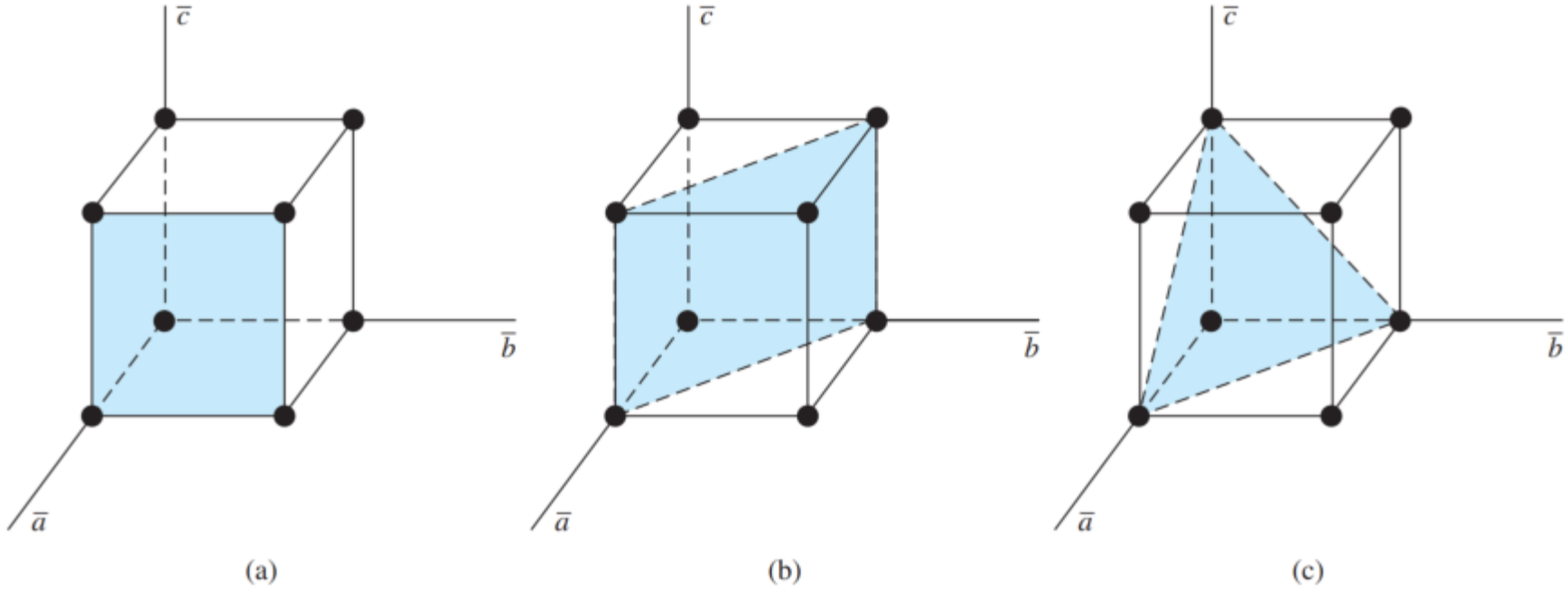


$$\vec{g} = p\vec{a} + q\vec{b} + s\vec{c} = 3\vec{a} + 2\vec{b} + 1\vec{c}$$

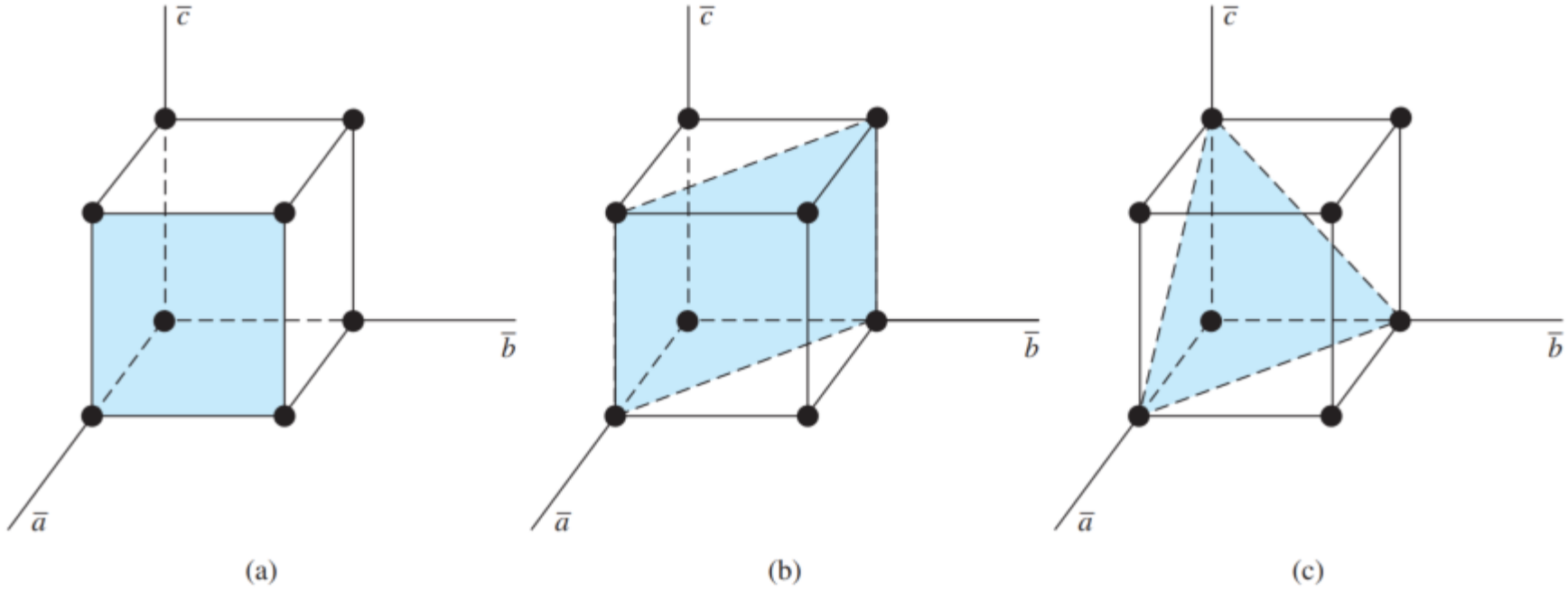
$$\left(\frac{1}{p}, \frac{1}{q}, \frac{1}{s}\right) = \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1}\right) = (2,3,6) = (236)$$

乘上三個分母的最小公倍數 6

Crystal Planes and Miller Indices



Crystal Planes and Miller Indices

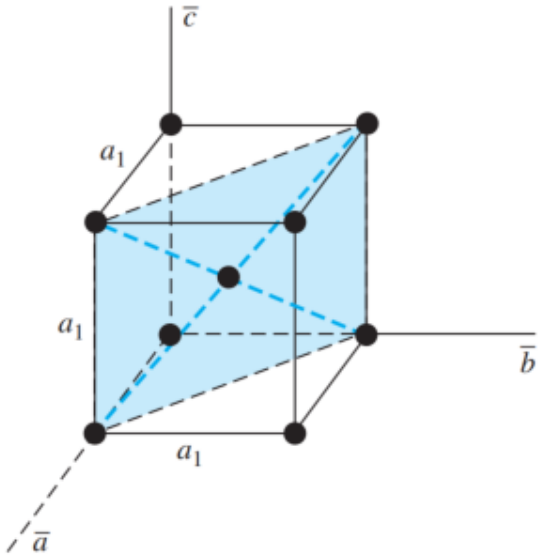


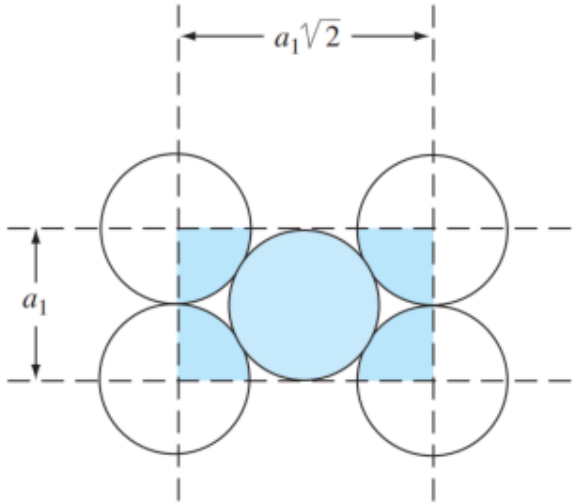
(100) (110) (111)

Example 1.3 Calculate the Surface Density

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 $a_1 = 5$ Å. Figure 1.9b shows how the atoms are cut by the (110) plane.



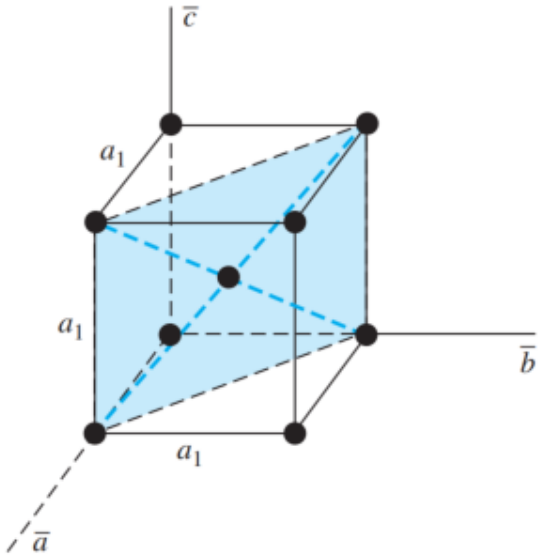


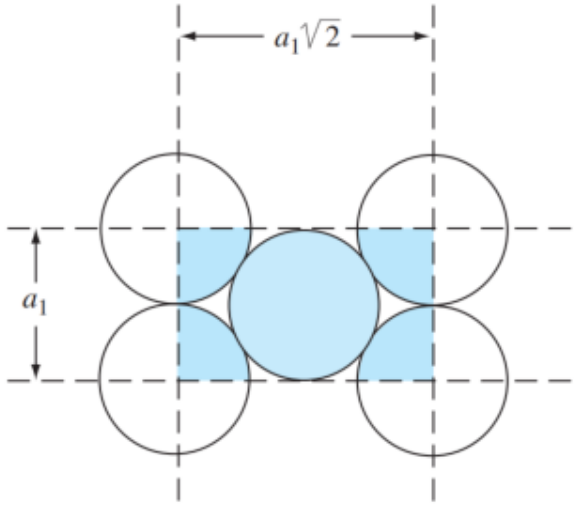
$$\text{Surface Density} = \frac{\#\ of\ atoms\ per\ lattice\ plane}{area\ of\ lattice\ plane}$$

Example 1.3 Calculate the Surface Density

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 $a_1 = 5$ Å. Figure 1.9b shows how the atoms are cut by the (110) plane.



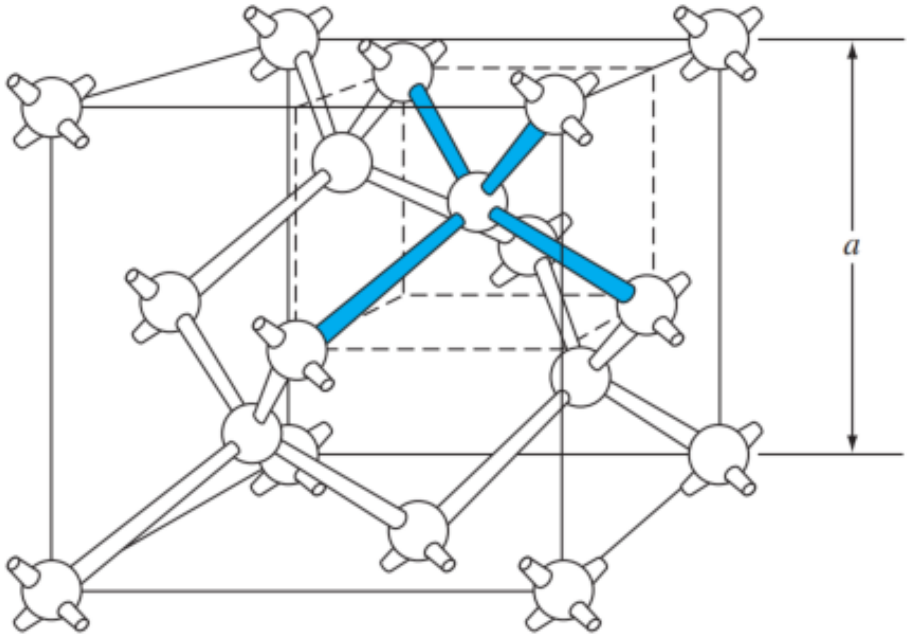


$$\frac{\left(4\times\frac{1}{4}+1\right)}{\left(5\times10^{-8}\right)\left(5\times10^{-8}\times\sqrt{2}\right)}=5.66\times10^{14}$$

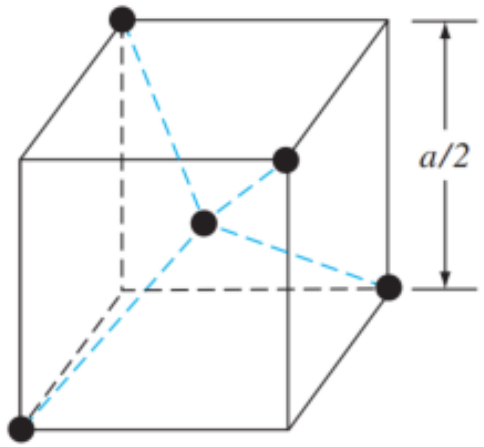
Atoms/cm^2

鑽石結構 The Diamond Structure

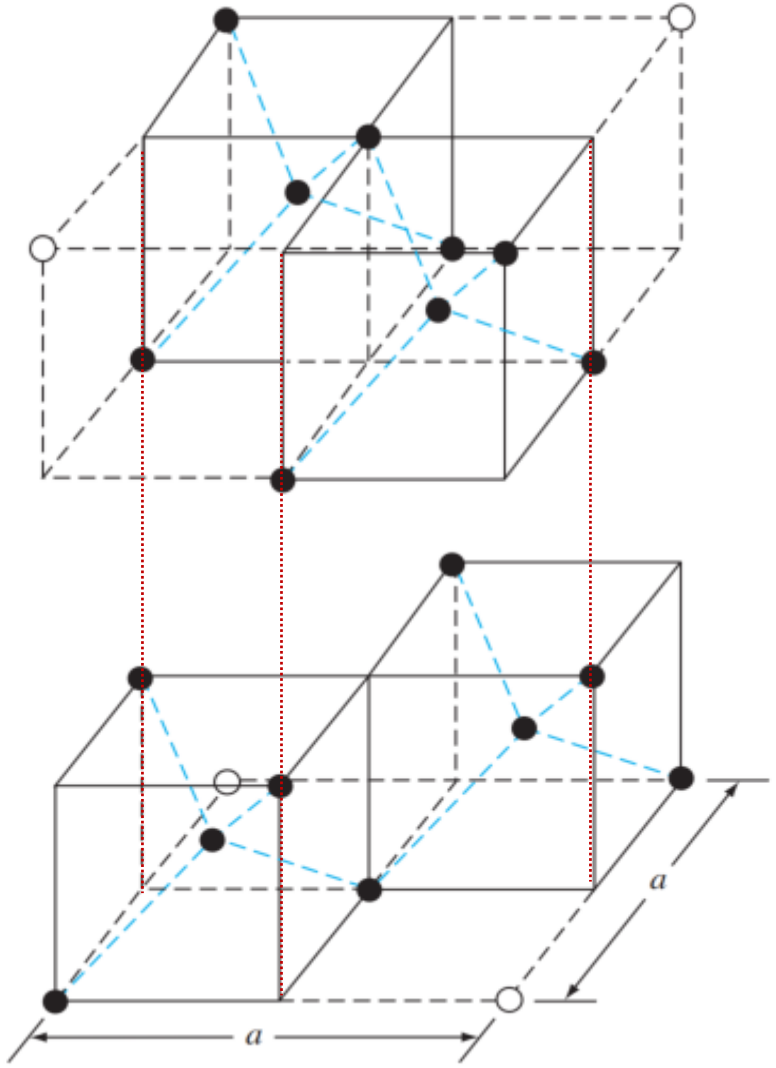
- 四面體 (tetrahedral structure)是一個體心立方去掉四個角落的原子組成。
- 鑽石結構基本上是由多個四面體 (tetrahedral structure) 組成的。



Tetrahedral structure

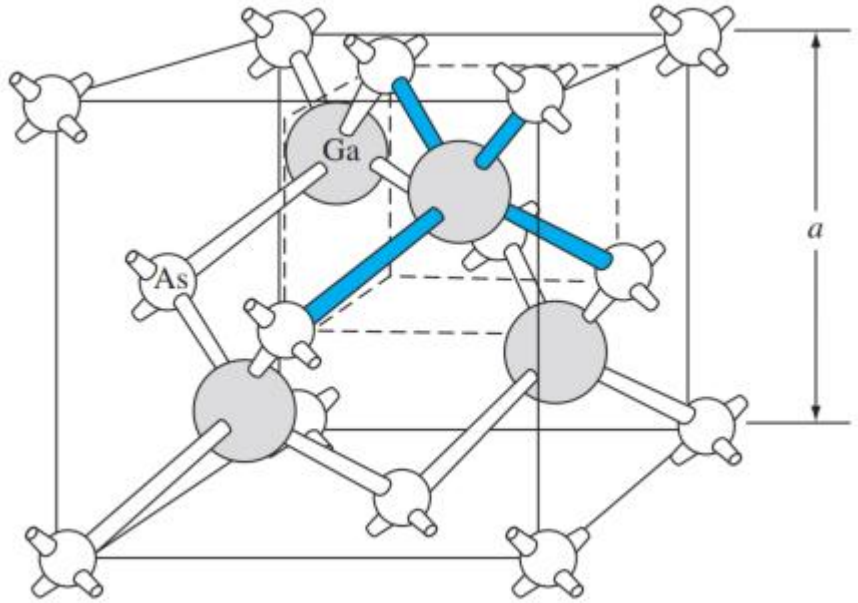


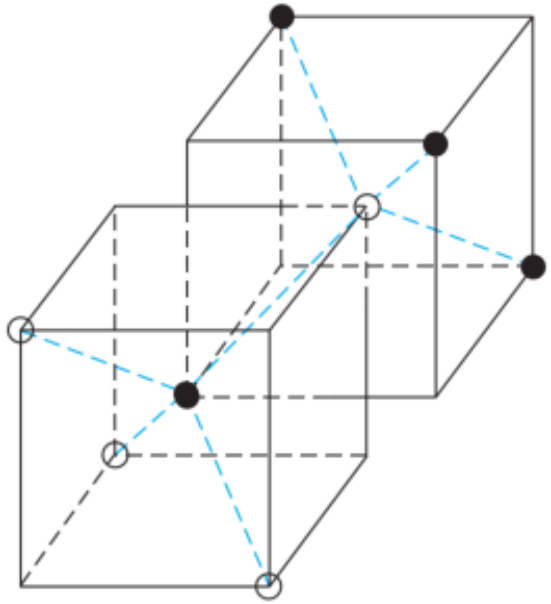
The Diamond Structure



閃鋅結構 Zincblende structure

- 閃鋅礦結構與金剛石結構的不同之處僅在於晶格中有兩種不同類型的原子
- 每個 Ga 原子有四個最近的 As 原子，每個 As 有四個最近的 Ga 原子。

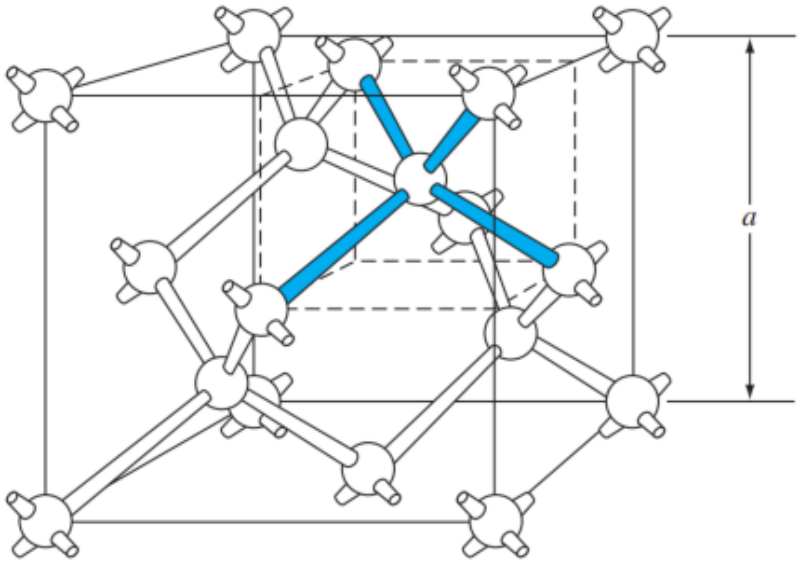




Test Your Understanding

TYU 1.4 Consider the diamond unit cell shown in Figure 1.11. Determine the (a) number of corner atoms, (b) number of face-centered atoms, and (c) number of atoms totally enclosed in the unit cell. [Ans. (a) 8; (b) 6; (c) 4]

TYU 1.5 The lattice constant of silicon is 5.43 Å. Calculate the volume density of silicon atoms. (Ans. 5×10^{22} cm^{-3})



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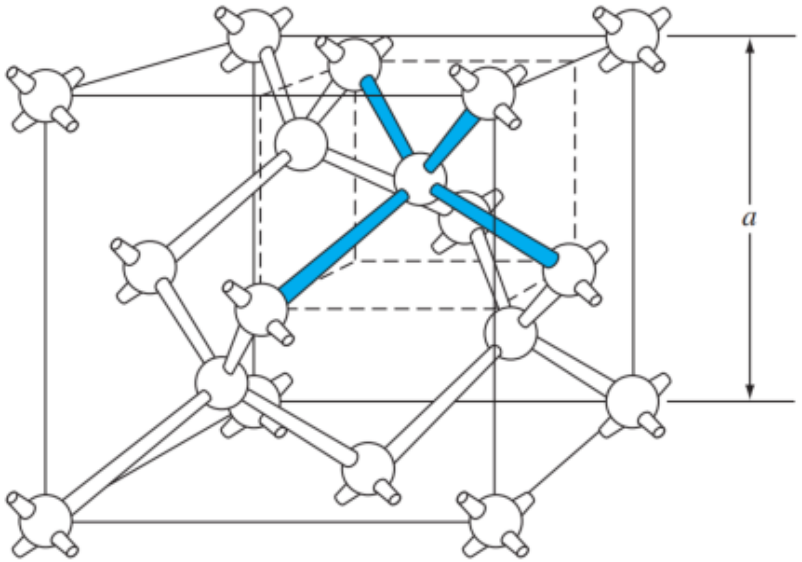
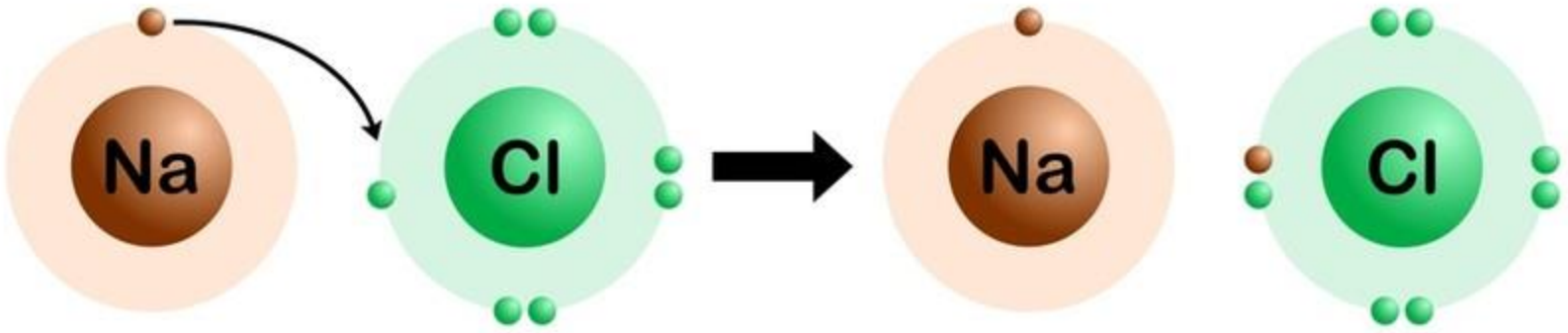


$$\frac{\left(8\times\frac{1}{8}+6\times\frac{1}{2}+4\right)}{\left(5.43\times10^{-8}\right)^{3}}=5\times10^{22}\quad \text{Atoms/cm}^3$$

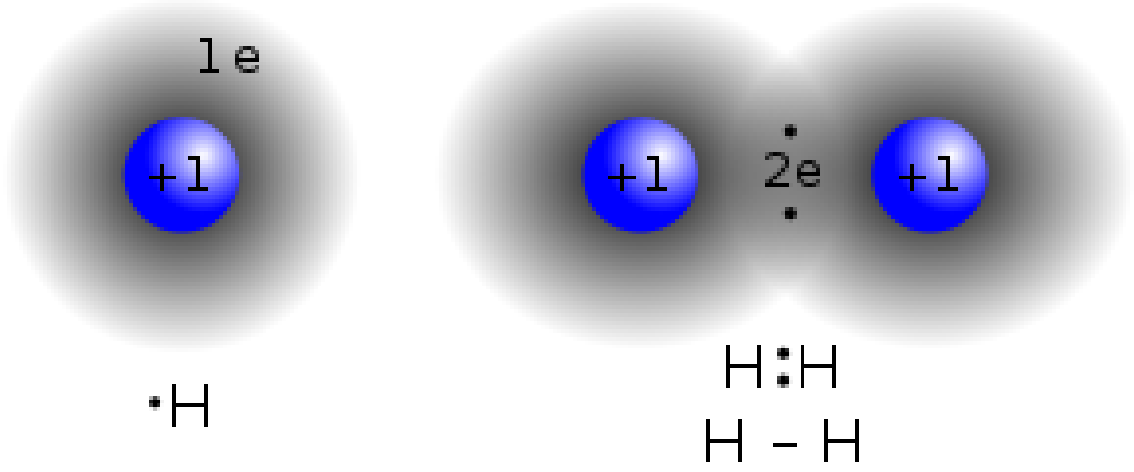
離子鍵 Ionic Bond

- 離子鍵通過兩個或多個原子失去或獲得電子而成為離子後形成。帶相反電荷的離子之間存在靜電吸引力，是離子化合物中主要交互作用。
- 此類經常是金屬與非金屬間形成，金屬元素失去電子，而非金屬元素得到電子。



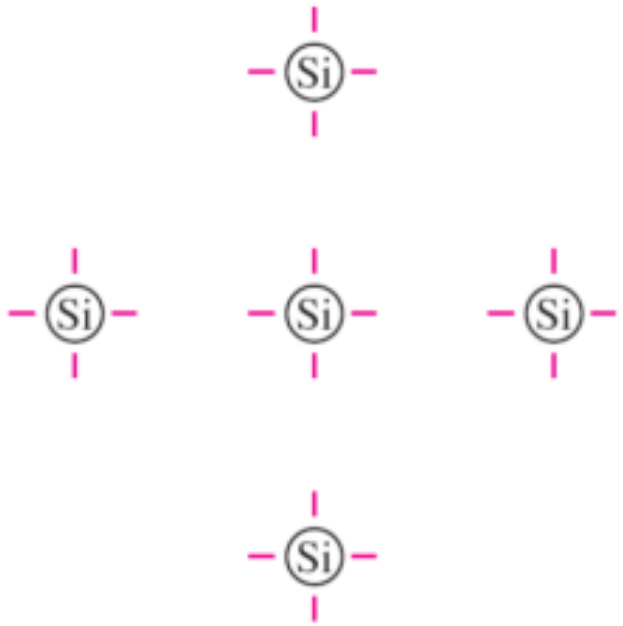
共價鍵 Covalent Bond

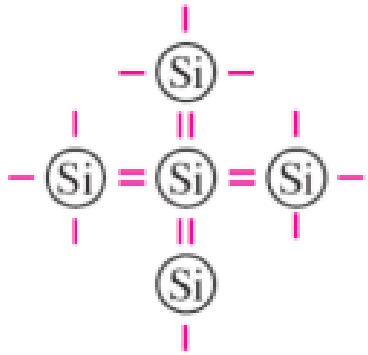
- 兩顆或以上非金屬原子共同使用它們的外層電子，在理想情況下達到電子飽和的狀態，由此組成比較穩定和堅固的化學結構。
- 與離子鍵不同，它們並沒有獲得或損失電子。同一種元素的原子或不同元素的原子都可以通過共價鍵結合，一般共價鍵結合的產物是分子，在少數情況下也可以形成晶體。



共價鍵 Covalent Bond

鄰近矽原子之間共享價電子，剛好滿足八隅體法則





金屬鍵 Metallic bond

- 游離電子與金屬離子之間的靜電吸引力組合而成。
- 由於電子是自由運動，金屬鍵沒有固定的方向，因而是非極性鍵。