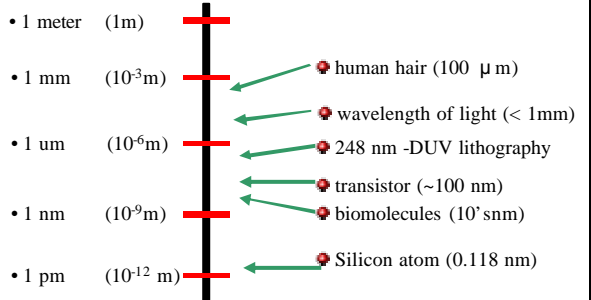


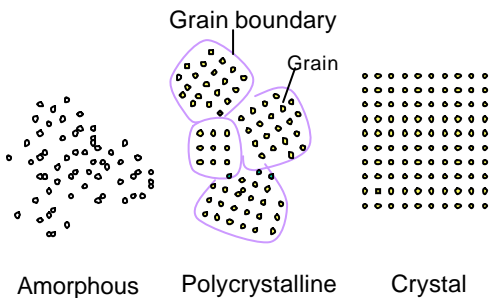
元件物理基礎

翁敏航
國家奈米元件實驗室 副研究員
mhweng@ndl.gov.tw

The scale of things

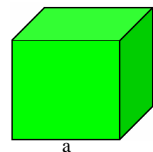
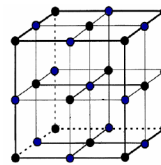


Crystal Structure



Crystal

- ❖ **Lattice** : The periodic arrangement of points in a crystal
- ❖ **Basis** : The constituent atoms attached to each lattice point
- ❖ **Crystal = Lattice + Basis**



a : Lattice constant

CRYSTAL STRUCTURES

> A direction of lattices plane

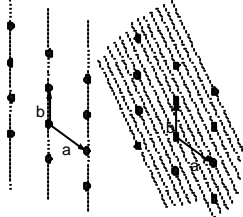


Fig. 10 (a) 二維晶格中的 (10) 平面 (b) 二維晶格中的 (32) 平面。

該講義部分內容非經翁敬航同意, 請勿擅自轉載使用

PRIMITIVE LATTICE

The basis consists of a primitive cell, arranging one cell at each lattice point will fill up the entire crystal without leaving undefined voids or overlapping regions. The Bravais lattice vectors describe how these repeating units in a crystal are tiled. A Bravais lattice can be defined as all points with positions

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad (6)$$

where \vec{a}_i are not in the same plane, and are n_i integers. The \vec{a}_i vectors are called the primitive vectors and there are many possible choices of these vectors.

該講義部分內容非經翁敬航同意, 請勿擅自轉載使用

System	Bravais lattice	Unit cell	Symmetry
Triclinic	Simple	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	None
Monoclinic	Simple Base-centered	$a \neq b \neq c$ $\alpha = \gamma = (\pi/2) \neq \beta$	One 2-fold rotation axis
Orthorhombic	Simple Base-centered Body-centered Face-centered	$a \neq b \neq c$ $\alpha = \beta = \gamma = (\pi/2)$	Three mutually orthogonal 2-fold rotational axis
Tetragonal	Simple Body-centered	$a=b \neq c$ $\alpha = \beta = \gamma = (\pi/2)$	One 4-fold rotation axis
Cubic	Simple Body-centered Face-centered	$a=b=c$ $\alpha = \beta = \gamma = (\pi/2)$	Four 3-fold rotation axis (along cube diagonal)
Trigonal	Simple	$a=b \neq c$ $\alpha = \beta = \gamma \neq (\pi/2)$	One 3-fold rotation axis
Hexagonal	Simple	$a=b \neq c$ $\alpha = \beta = (\pi/2)$ $\gamma = (2\pi/3)$	One 3-fold rotation axis

該講義部分內容非經翁敬航同意, 請勿擅自轉載使用

CRYSTAL STRUCTURES

> Cubic $a=b=c$ $\alpha = \beta = \gamma = (\pi/2)$

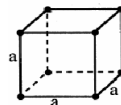


Fig. 5(a)

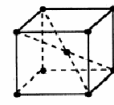


Fig. 5(b)

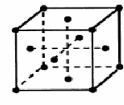


Fig. 5(c)

> Tetragonal

$a=b$

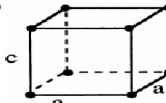


Fig. 5(d)

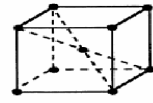


Fig. 5(e)

該講義部分內容非經翁敬航同意, 請勿擅自轉載使用

CRYSTAL STRUCTURES

➤ Orthohombica $b = c \neq a$ ($\neq \sqrt{2}$)

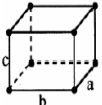


Fig. 6(a)

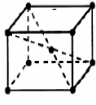


Fig. 6(b)

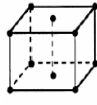


Fig. 6(c)

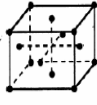


Fig. 6(d)

➤ Hexagonal $a = b \neq c$ ($\neq \sqrt{2}$)
 $\neq (2/\sqrt{3})$

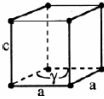


Fig. 6(e)

該講義部分內容非經翁敏航同意,請勿擅自轉載使用

CRYSTAL STRUCTURES

➤ Trigonal $a = b = c$ ($\neq \sqrt{2}$)

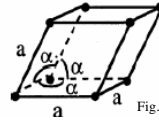


Fig. 7(a)

➤ Monoclinic $b \neq a \neq c$ ($\neq \sqrt{2}$)

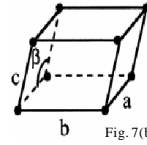


Fig. 7(b)

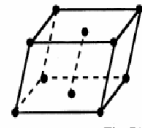


Fig. 7(c)

該講義部分內容非經翁敏航同意,請勿擅自轉載使用

CRYSTAL STRUCTURES

➤ Triclinic $a \neq b \neq c$

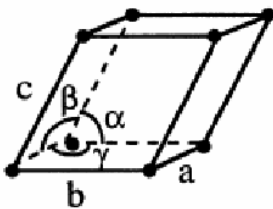
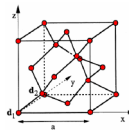


Fig. 8

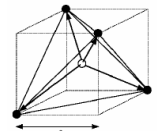
該講義部分內容非經翁敏航同意,請勿擅自轉載使用

Crystal Structure

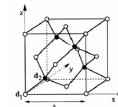
➤ Diamond Structure (Ex: Si) ➤ Unit Cell in Diamond & Zincblende Structure



Atom 1



➤ Zincblende Structure (Ex: GaAs)



Atom 1

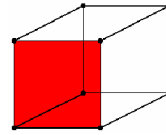
Atom 2

Miller Indices

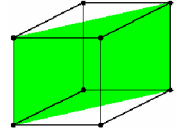
❖ The Miller indices are obtained using the following steps.

- Find the intercepts of the plane on the three Cartesian coordinate in terms of the lattice constant.
- Take the reciprocals of these numbers and reduce them to the smallest three integers having the same ratio.
- Enclose the result in parentheses (hkl) as the Miller indices for a single plane.

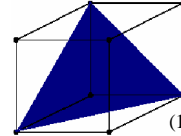
Miller Indices



(100)面

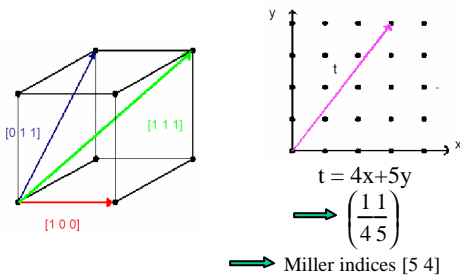


(110)面



(111)面

Miller Indices



RECIPROCAL LATTICE

The reciprocal lattice can be defined as all that satisfy

$$\vec{k} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3 \quad (7)$$

The \vec{b}_i vectors are generated by satisfying the following

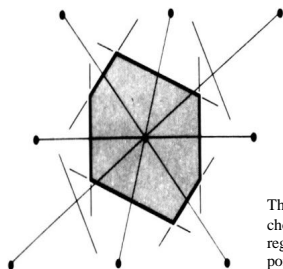
relation: $\vec{k} \cdot \vec{R} = (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3) \cdot (m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3) = N \cdot 2\pi$ (8)

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad (9)$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} \quad (10)$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)} \quad (11)$$

WIGNER-SEITZ CELL

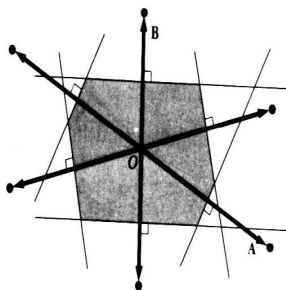


決定一原始晶胞：(1)選擇一個晶格點用直線與它附近晶格點連接起來；(2)劃出這些連接線的垂直平分線(或面)。用這種方法所得到的最小封閉體積稱為威格納-賽茲原始晶胞，所有空間都可用這些晶胞填滿。

The Wigner-Seitz cell is the most common choice for the primitive unit cell. This defines a region of space that is closer to a particular point rather than to any other point on a Bravais lattice.

該講義部分內容非經翁敏航同意，請勿擅自轉載使用

THE FIRST BRILLOUIN ZONE



二維斜晶格的第一布里淵區的構圖。在倒晶格中，首先由O點到鄰近諸點畫出一些向量，然後再畫出這些向量的垂直平分線，而所圍起來的最小區域就是第一布里淵區。

該講義部分內容非經翁敏航同意，請勿擅自轉載使用

BRAGG REFLECTION

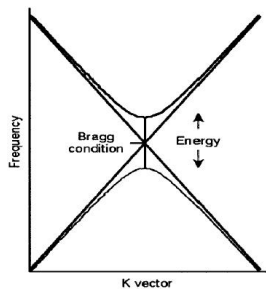


Fig. Plot showing an example of the dispersion relation and the Bragg condition.

In such forbidden frequency gaps or "Bragg frequencies," electromagnetic waves attempting to propagate experience exponential attenuation due to Bragg reflections. Although it has been shown that omnidirectional reflection can be achieved with a one-dimensional periodicity, this is only true when the point source of waves is not placed close to the crystal structure.

該講義部分內容非經翁敏航同意，請勿擅自轉載使用

BRAGG CONDITION

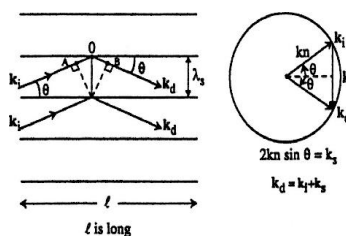


Fig. θ is the angle of incidence, which is also the angle of diffraction

該講義部分內容非經翁敏航同意，請勿擅自轉載使用

X光晶體學

The Bragg law :

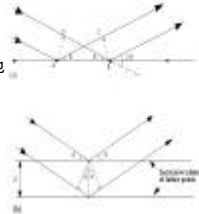
■ 一般X光的波長約在1埃附近，該長度也正好接近固體內原子與原子間的距離。

$$\rightarrow 2d \sin \theta = n\lambda$$

其中d為平面與平面間之距離，而n為整數。這也就所謂Bragg's Law。

■ 根據Bragg's Law並不是任何平面都可以產生所謂的繞射現象，只有符合特殊的入射角度以及入射波長的X光才有可能出現。

Bragg's Law的證明 (a) 同一平面之原子，若反射之電磁波對於原子A與原子B有波程差而且是整數倍，將會產生強烈干涉。(b) 不同平面的原子，亦有可能產生同樣之結果。

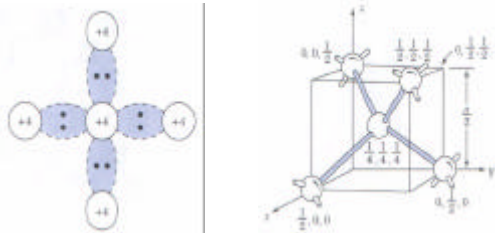


半導體材料

- 目前半導體材料中最常見的有矽、鎢以及砷化鎵等等，前者屬於鑽石結構，而後者屬於Zincblende 結構。
- 結構多半都屬於共價鍵的鍵結。
- 在絕對溫度為零時，其最高能量之能帶都填滿了電子，由於這些電子是參與鍵結用，是屬於價電子，因此這些價電子所存在的能帶，我們稱之為價電帶 (valence band)。
- 至於那些未被電子佔有的能帶，由於一旦有電子進入便可以產生導電的效果，因此我們賦予導電帶 (conduction band) 的名稱。價電帶與導電帶之間有一間隙，我們稱之為能隙。
- 對於一般半導體而言大約在1eV附近。半導體真正的表現是完全決定在靠近在價電帶以及導電帶附近的電子。

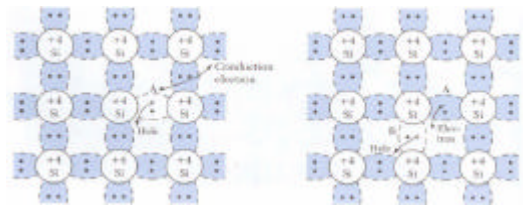
Si Crystal

■ In crystal structure , atoms shares their valence electrons with its neighbors. These sharing of electrons is covalent bonding.



電子 & 電洞

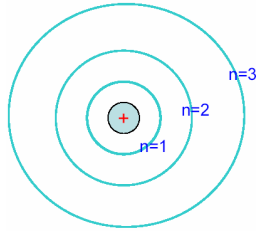
■ At higher temperature, thermal vibration may break the covalent bonds; the free electrons can participate in current conduction. When electrons leave the covalent bond, the vacancies were considered as a particle similar to an electron. This fictitious particle is called a hole.



Hydrogen Atomic Model

Bohr's Model :

$$E_H = \frac{-m_e q^4}{8 \epsilon_0^2 h^2 n^2}$$



Hydrogen Atomic Model

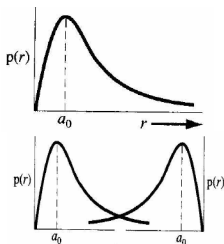
■ For an atom, each electron must have a separate distinct energy state defined by 4 quantum numbers:

- A. Principle quantum number, $n = 1, 2, 3$
- B. Angular momentum quantum number, $l = 0, 1, 2, \dots, n-1$
- C. Magnetic quantum number, $m = 0, \pm 1, \dots, \pm l$
- D. Electron spin, $s = \pm 1/2$

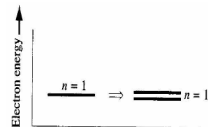
■ Only hydrogen atom can be solved due to electron-electron interaction

Band Formation

■ The interaction results in the discrete quantized energy level splitting into two discrete energy levels.

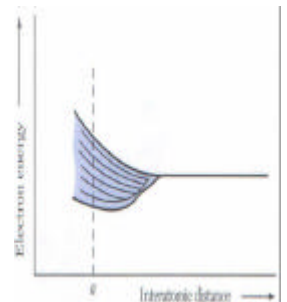


Probability density function of a isolated hydrogen atom

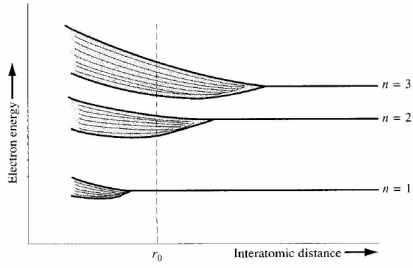


Energy Band

■ Degenerate :
When N isolated atoms are brought together to form a solid, the orbits of the outer electrons of different atoms overlap and interact with each other.



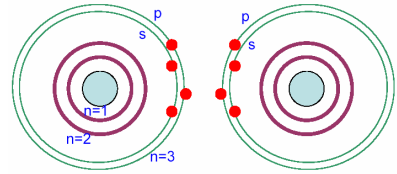
Energy Band



Schematic showing the splitting of three energy states into allowed bands of energies.

Band Formation

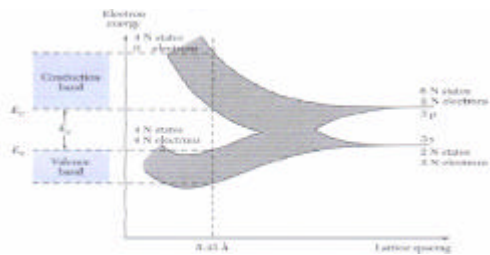
p orbital : six allowed states
s orbital : two allowed states



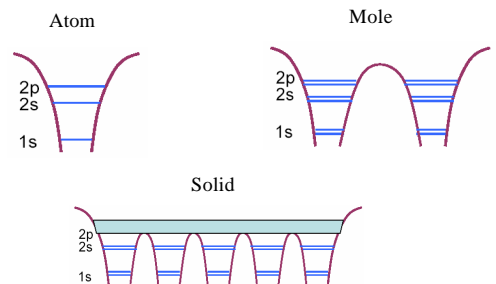
Si Atom Interaction

Band Formation

■ Schematic diagram of the formation of a silicon crystal from N isolated silicon atoms.

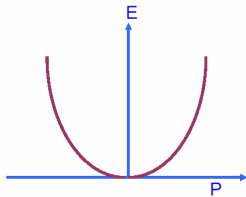


Band Formation



Energy Momentum Diagram

- For a free electron, energy E can be given by :



$$E = \frac{P^2}{2m_0}$$

m_0 : effective mass
 P : momentum

Effective Mass Concept

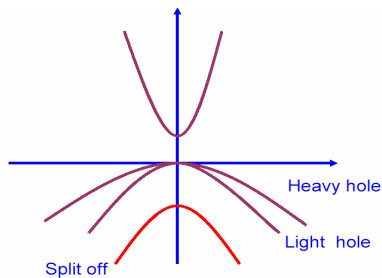
- Electrons in conduction band and holes in valence band are similar to free electrons since they can move relatively freely.
- We can treat electrons and holes as classical particles.

$$E = \frac{\vec{P}^2}{2m_n} \quad m_n = \left[\frac{d^2 E}{d^2 p} \right]^{-1}$$

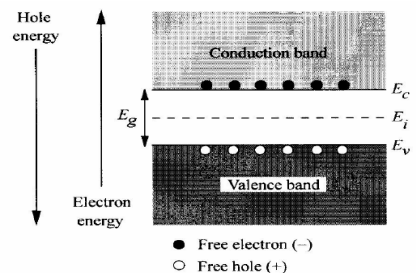
m_n : effective mass

\vec{P} : crystal momentum of electron

Effective Mass Concept



Energy Band Diagram of Silicon



Energy Band

➤ Temperature Effect :

◆ Band Gap vs. Temperature

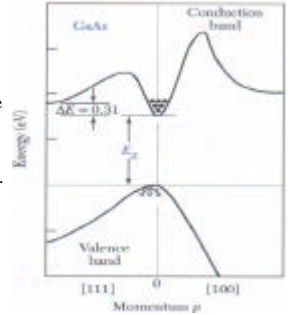
$$E_g(T) = 1.17 - \frac{(4.73 \times 10^{-4})T^2}{(T + 636)} \quad \blacklozenge \text{ Si}$$

$$E_g(T) = 1.52 - \frac{(5.4 \times 10^{-4})T^2}{(T + 204)} \quad \blacklozenge \text{ GaAs}$$

Band Structure

➤ Direct Semiconductor

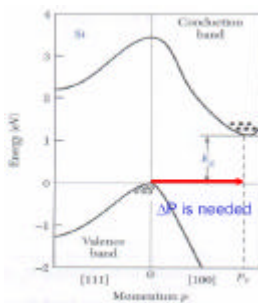
■ The top of the highest (occupied) valence band and the bottom of the lowest (unoccupied) conduction band are at the same value in k-space. In most cases this k-point is the origin of the BZ, the G point. Examples: GaAs, InP, GaN, ZnO.



Band Structure

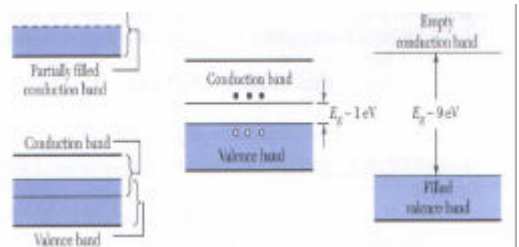
➤ Indirect semiconductor:

■ The extreme at the top of the valence band and at the bottom of the conduction band are at different k-values. Examples: Ge, Si.



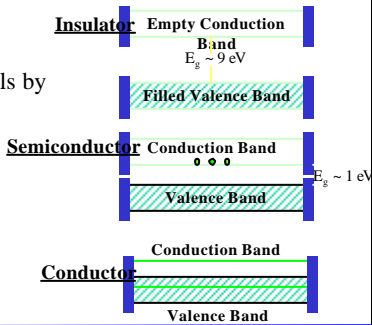
Energy Band

➤ Conductor, Semiconductor & insulator



Conductivity of Materials

- 3 types of materials by their electrical conductivity
 - Insulator
 - Semiconductor
 - Conductor



Intrinsic Carrier Concentration

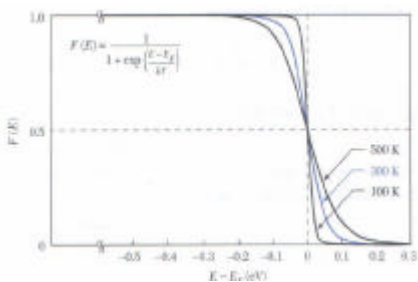
- Intrinsic Semiconductor is one that contains relatively small amounts of impurities compared with the thermally generated electrons and holes.
- Fermi-Dirac Distribution Function.

$$F(E) = \frac{1}{1 + e^{(E - E_f) / kT}}$$

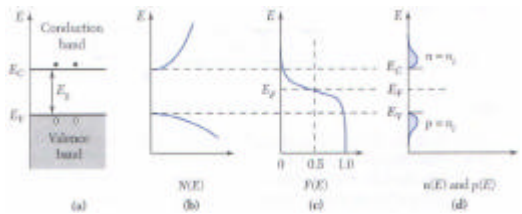
$$F(E) \cong e^{-(E - E_f) / kT} \text{ When } (E - E_f) > 3kT$$

$$F(E) \cong 1 - e^{-(E - E_f) / kT} \text{ When } (E - E_f) < -3kT$$

Intrinsic Carrier Concentration

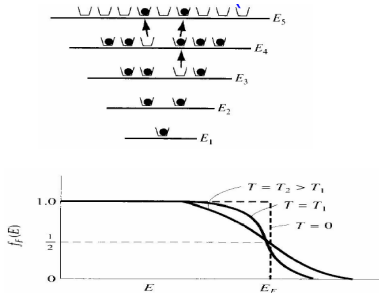


Intrinsic Carrier Concentration



Intrinsic semiconductor. (a) Schematic band diagram. (b) Density of states. (c) Fermi distribution function. (d) Carrier concentration.

Thermal Excitation ($T > 0 \text{ K}$)



Fermi-Dirac Distribution

$$\frac{N(E)}{g(E)} = f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

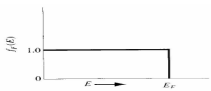
➤ Probability that a quantum state at the energy E will be occupied by an electron

$$T = 0 \quad E > E_F \quad f_F(E) = 0$$

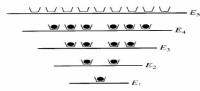
$$E < E_F \quad f_F(E) = 1$$

$$T > 0 \quad E = E_F \quad f_F(E) = \frac{1}{2}$$

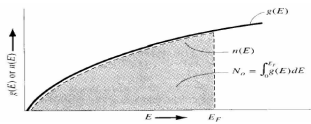
Fermi Level at $T = 0 \text{ K}$



The Fermi probability function versus energy for $T = 0 \text{ K}$

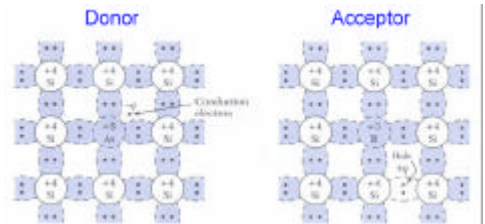


Discrete energy states and quantum states for a particular system at $T = 0 \text{ K}$



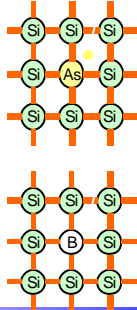
Donor & Acceptor

➤ **Extrinsic** : A semiconductor doped with donor or acceptor impurities.



N- and P- Doped

- Increase the conductivity of the semiconductor with impurity
- N- (As, P): donate electrons
 - As⁺, P⁺
 - Majority carrier : electron
 - Minority carrier : hole
- P- (B)
 - B⁻
 - Majority carrier : hole
 - Minority carrier : electron



Intrinsic Carrier Concentration

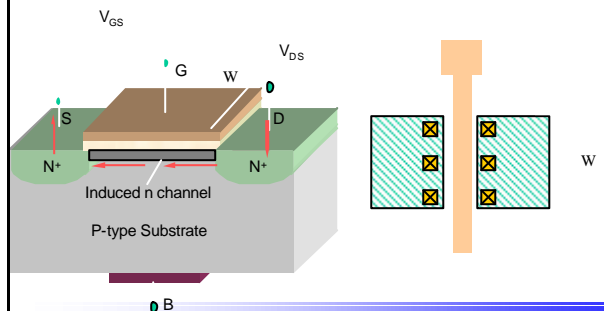
- 在純的半導體晶體中 (也就是沒有雜質在晶體內) 電子與電洞的數目式相同的。
- 電洞的產生是由價電帶的電子受到熱能之故，跳躍到導電帶之下所形成的，因此每當導電帶多一個電子則價電帶便產生一個電洞。
- 矽與鍺半導體在常溫時其本質的載子濃度分別為 2×10^{16} 以及 $2 \times 10^{19} \text{ m}^{-3}$ 。
- 任何半導體其本質載子的濃度可以寫成

$$np = n_i^2(T)$$
- 其中 n_i 會隨著溫度增加而增加。

Extrinsic Carrier Concentration

- 載子的濃度完全是被施體雜質的濃度所掌控，由於是電子濃度多餘電洞濃度我們稱該半導體為n型半導體，電子為多數載子，而電洞為少數載子
- 反之若受體雜質的濃度超過施體雜質的濃度時，則該半導體內電洞的濃度將超過電子濃度，此時該半導體稱之為p型半導體
- 半導體的施體雜質在室溫時，大部分都會游離，因此電子的濃度可以被預估，而電洞的濃度則由 law of mass action來求得

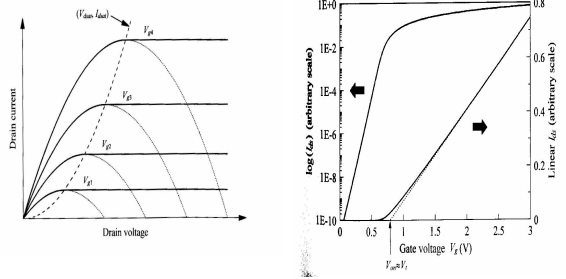
Metal-Oxide-Silicon Field Effect Transistor MOSFET



I-V Characteristics of a MOSFETs

- Threshold Voltage (V_T):
 - V_T is the gate bias which make substrate start to inverse strongly
- $V_G > V_T$: dominated by drift current
 - Linear Region _____
 - Saturation Region _____ "ON" State
- $V_G < V_T$: dominated by diffusion current
 - Subthreshold _____
 - _____ "OFF" State

I-V Characteristics of a MOSFETs



MOSFET

- MOS的結構，主要包含半導體、金屬與氧化層
 - 半導體層直接由晶圓之底材矽組成
 - 氧化層（即 SiO_2 ）可以氧化爐管(Oxidation Furnace)製造
 - 金屬層必須以氣相沈積（Vapor Phase Deposition）來製作，尤其是CVD法或濺鍍法。
 - 位於閘極兩旁的源極與汲極，同樣都是以矽為主的半導體層，不過其極性與底材矽相反，因此必須選擇性地對此兩區域進行摻雜（Doping），通常使用離子植入法(Ion Implantation)或熱擴散法（Thermal Diffusion）

MOSFET

- 隔離製程(Isolation Process)
 - 在積體電路，為了使電晶體與電晶體間的操作不至於受到對方的干擾，必須設法將積體電路上的電晶體與其他電晶體相隔離，以避免產生短路。
- 區域氧化法(Local Oxidation, LOCOS)
 - 其原理是利用熱氧化法，選擇性地在電晶體與電晶體之間，長出一層厚度約連數千埃的二氧化矽層。利用其之非導電性來執行MOS電晶體間之隔離功能，此層隔離用之氧化層被稱為場氧化層（Field Oxide）
- 溝渠隔離(Trench Isolation)
 - 此為新一代記憶體製程的CMOS隔離技術。
 - 其原理為利用非等向性(Anisotropic)乾蝕刻，我們可在PMOS與NMOS之間開出一道溝渠，然後把它陸續填入二氧化矽及多晶矽。若此溝渠之深度超過CMOS之井深，CMOS裡的PMOS及NMOS將被成功的隔離。
- 絕緣層上矽法(Silicon On Isolation, SOI)
 - 其原理是在底材矽的表面不遺處，增加一層絕緣體（通常為二氧化矽），讓用以製作CMOS元件的底材矽與矽主體之間，以這一層絕緣層加以隔開。
 - 因為建築CMOS的區域並不與底材相連，因此CMOS電晶體發生閉鎖的一些途徑，如源極與底材、井與底材等的連結，將因為中間這層絕緣層的隔離而消失，使閉鎖現象不在存在。

MOSFET

- 通道阻絕層(Channel Stop)
 - 大多數的金屬線跨過數量不等的氧化層，執行其作為元件間的導線的功能。因為二氧化矽是一種介電材料，任何具電壓的金屬線與其相接觸，都會像MOS電容一般地，在二氧化矽場氧化層的下方（即底材矽），聚集一定量的電荷（ $Q = CV$ ）。
 - 因為這些在場氧化層下方因電容效應所產生的電荷會影響到鄰近電晶體的隔離效果，為了避免這些產生電荷的密度太高而發生氧化層隔離失效的問題，我們通常在場氧化層的正下方，以離子植入或是熱擴散的方式，摻入一定濃度，且與底材極性相同的摻質來進一步保障場氧化層的隔離能力。
 - 這層在底材表面，以摻雜的方式製作的區域，我們通常稱之為通道阻絕層。

MOSFET

- 短通道效應
 - MOS元件越小，通道的長度將隨之縮短，因此電晶體的操作速度將加快。但是電晶體的通道長度並不能無限制的縮減，當其長度縮短到某一定的程度後，各種因通道長度變小所衍生的問題便會發生，這種現象稱為短通道效應（Short Channel Effects）
 - 假如我們保持MOS所有參數設計不變，緊縮短MOS的通道長度設計（通道長度指的是源極及汲極在半導體表面所相隔的距離），MOS在操作時於源極和汲極所產生的缺乏層，將與通道產生重疊。而且通道長度越短，其與MOS源極與汲極的缺乏層寬度就越接近，產生重疊的比例將越高。
 - 因為部份通道被源極及汲極得缺乏層共享，**次啟始電流(Subthreshold Current)**將上升，使得MOS的 V_t 下降，甚至使得 V_g 無法對MOS的汲極電流 I_d 做控制的情形出現
 - 當MOS的通道長度縮短之後，除了會造成 V_t 的下降與 V_g 對MOS電晶體的控制發生問題以外，另一種稱為**熱電子效應(Hot Electron Effect)**的現象，也會隨著通道長度的縮短而影響MOS電晶體的操作。

MOSFET

- 熱電子效應
 - 當NMOS電晶體的通道長度縮小，若施加的電壓大小不變，通道內的橫向電場將增加（電場 = 電壓/長度），這將使得通道內的電子藉由電場加速所獲得的能量上升，尤其是在通道的汲極相接的附近，電子能量將很高。
 - 汲極附近處於價帶的電子，有機會因為被這些熱電子所撞擊而提升至導帶，而產生許多的電子-電洞對。所以當NMOS的通道縮短，通道接近汲極地區的載子數量將上升。這個現象稱為**載子倍增**。
 - 載子倍增所產生的電子，通常吸往汲極（ $V_d > 0$ ），而增加汲極的電流大小。
 - 部份電子足以射入閘氧化層裡；而所產生之電洞將流往底材，而產生底材電流；另一部份的電洞則被源極所收集，這使得npn現象加強，熱電子的數量增加，促使更多載子倍增，甚至進而發生電崩潰（Electrical Breakdown）的情形。

MOSFET

- 輕微摻雜汲極法（Lightly Doped Drain, LDD）
 - 所謂LDD法乃是在原來的MOS的源極和汲極接近通道的地方，在增加一組摻雜程度較原來n型的源極與汲極為低的n型區。
 - 有LDD設計的MOS的電場分布，將往汲極移動，且電場的大小也將比無LDD的MOS為低。因此熱電子效應便可以被減輕。
 - 另外部份電子跨過氧化層界面而往閘極前進，這些電子大多陷於氧化層內，使得氧化層的電荷改變，其將隨著MOS的操作而增加，而LDD的設計，也可減少這類問題的發生。