

# Semiconductor Devices

## PH 205



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### Syllabus

**Physics:** Energy bands in solids and Charge carriers. Semiconductors: Elemental and compound semiconductors, intrinsic and extrinsic materials, Direct and indirect band-gap semiconductors, Heavily doped semiconductors. Charge carrier in semiconductors: mobility, impurity band conduction, nonlinear conductivity, excess carriers in semiconductors. Semiconductor Bloch equation, transport properties.

**P-N junctions:** fabrication, static and dynamic behavior of p-n junction diodes, Junction breakdown in p-n junctions, tunnel diode, Schottky diode.

**Metal Semiconductor junctions:** Schottky effect, rectifying and Ohmic contacts. Integrated circuits, fabrication methods

**Optoelectronic Devices:** photodiodes, light emitting diodes, semiconductor lasers, photovoltaic cells

**Bipolar Junction Transistor:** fundamentals of BJT operation, BJT fabrication, carrier distribution and terminal current, generalized biasing, switches, frequency limitations of transistors. Field Effect Transistors: JFET, MOSFET.

**Texts:**

1. S. M. Sze, *Physics of Semiconductor devices*, 2nd Ed., John Wiley, 1982.
2. **J. Singh, *Semiconductor Devices - Basic Principles*, John Wiley, 2001.**

**References:**

1. M. S. Tyagi, *Introduction to Semiconductor Materials and Devices*, John Wiley, 2008.
2. B. G. Streetman, *Solid State Electronic Devices*, 5th Ed., PHI, 2001.

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## Evaluation Scheme

- Quizes: 2 nos (10 marks each)
- Mid-sem: 30 marks
- End-sem: 50 marks
- Attendance & class response
- Relative grading

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**Properties that gives Semiconductors unique abilities to produce intelligent devices**

**Band structure:**  
Valence band, conduction band and region of forbidden bandgap

Controlled introduction of dopants/impurities to alter material conductivity by up to 10 orders of magnitude

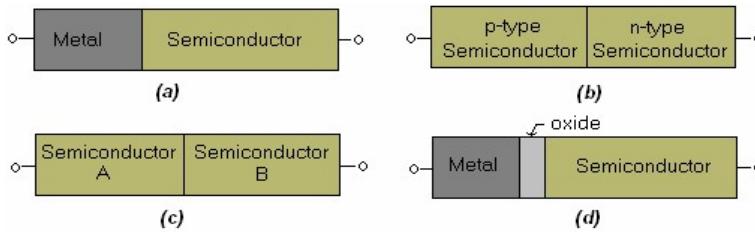
Isolation of regions of a device and electrical contacts

Small dimensional structures for high speed/high density

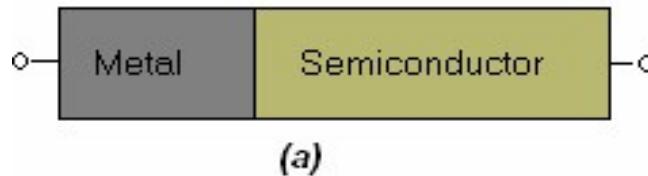
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## Device Building Blocks

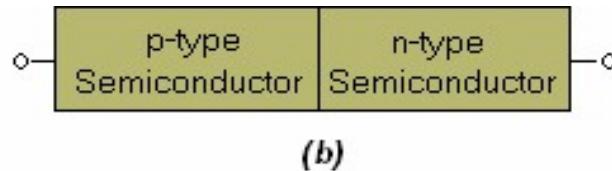
- Semiconductor devices have been studied for over **130 years**.
- About 60 major devices with over 100 device variations related to them.
- All these devices can be constructed from a small number of **device building block**.



- **Fig.1:** Basic device building blocks. (a) Metal-semiconductor interface; (b) *p-n* junction; (c) heterojunction interface; (d) metal-oxide-semiconductor structure(MOS).

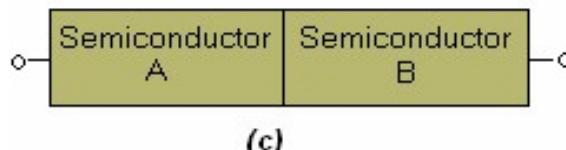


- Figure 1a is a metal-semiconductor interface, which is an intimate contact between a metal and semiconductor.
- This building block was the first semiconductor device ever studied in 1874.



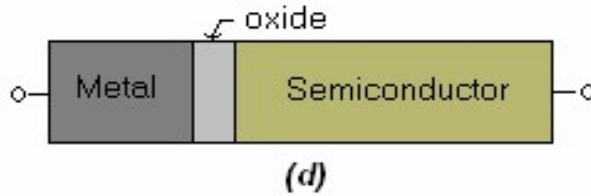
(b)

- The second building block is the p-n junction (Fig1b), formed between a p-type (with positively charged carriers) and an n-type (with negatively charged carriers) semiconductors.
- The p-n junction is a key building block for most semiconductor devices.



(c)

- The third building block (Fig1c), is the **heterojunction interface**, an interface formed between two dissimilar semiconductors.
- the key components for high-speed and photonic devices.

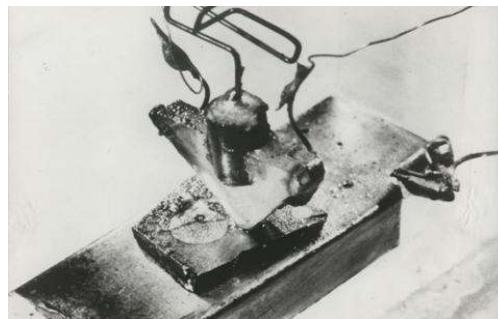


- Figure 1d shows the **metal oxide semiconductor (MOS)** structure.
- The structure can be considered a combination of a metal-oxide interface and an oxide-semiconductor interface.

## Major Semiconductor Devices: History

- **1874:** **metal-semiconductor contacts** studied by **Braun**, who discovered that the **resistance** of contacts between metals and metal sulfides (e.g., copper pyrite, CuS) **depended on** the magnitude and **polarity of the applied voltage**.
- **1907:** The electroluminescence phenomenon (for the **light-emitting diode**) was discovered by **Round**. He observed the generation of yellowish light from a crystal of carborundum (**SiC**) when he applied a potential of 10 V between two points on the crystals.
- **1947:** **The point-contact transistor** was invented by **Bardeen and Brattain**.

- **1949:** This was followed by Shockley's classic paper on ***p-n junction*** and **bipolar transistor** which is a key semiconductor device (Fig. 2).



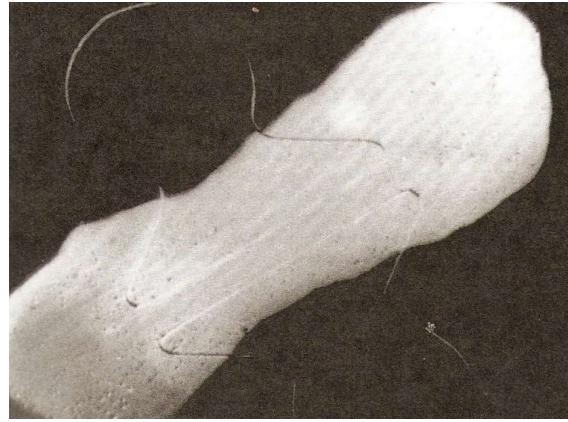
*a centimeter long!*

Fig.2 The first transistor. (Photograph courtesy of Bell Laboratories)

- **1952:** Ebers developed the basic model for the **thyristor**, which is an extremely versatile switching device.
- **1954:** The **solar cell** was developed by Chapin, et al. using a silicon *p-n* junction. The solar cell is a major candidate for obtaining energy from the sun because it can convert sunlight directly to electricity and is environmentally benign.
- **1957:** Kroemer proposed the **heterojunction bipolar transistor** to improve the transistor performance.
- **1958:** Esaki observed negative resistance characteristics in a heavily doped *p-n* junction, which led to the discovery of the **tunnel diode** which is important for ohmic contacts and carrier transport through thin layers.
- **1960:** The most important device for advanced integrated circuits is the **MOSFET**, which was reported by Kahng and Atalla.
- Figure 3 shows the first device using a **thermally oxidized silicon** substrate. The device has a gate length of 20  $\mu\text{m}$  and a gate oxide thickness of 100 nm.

The MOSFET and its related integrated circuits now constitute about **90% of the semiconductor device market.**

An ultrasmall MOSFET with a **channel length of 20 nm** had been demonstrated in **2001** which can serve as the basis for the most advanced integrated chips containing over one trillion ( $>10^{12}$ ) devices



**Fig.3 The first metal-oxide semiconductor field-effect transistor MOSFET (Photograph courtesy of Bell Laboratories, USA.)**

- **1962:** Hall et al. first achieved lasing in semiconductors.
- **1963:** Kroemer, Alferov and Kazarинов proposed the heterostructure laser. These proposals laid the foundation for modern laser diodes, which can be operated continuously at room temperature. Laser diodes are the key components for a wide range of applications, including digital video disk, optical fiber communication, laser printing, and atmospheric-pollution monitoring. During this year, Gunn invented transferred-electron diode which is used in such millimeter-wave applications as detections systems, remote controls, and microwave test instrument.
- **1965:** IMPATT diode's operation was first observed by Johnston et al. They can generate the highest continuous wave (CW) power at millimeter-wave frequencies of all semiconductor devices. They are used in radar and alarm systems.

- **1966:** Mead invented **MESFET** which is a key device for monolithic microwave integrated circuits (MMIC).
- **1967:** Kahng and Sze invented the **nonvolatile semiconductor memory (NVSM)** which can retain its stored information when the power supply is switched off. A schematic diagram of the first NVSM is shown in Fig.4a.

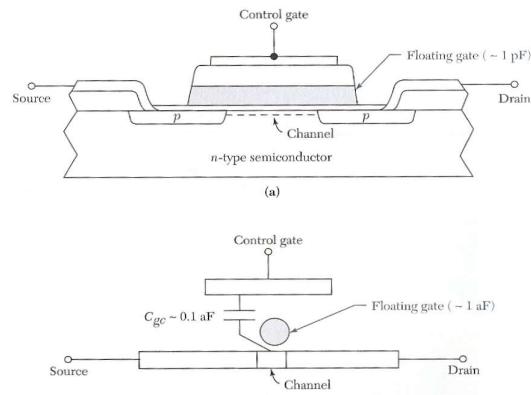


Fig.4

- **1994:** The operation of a SEMC ( a limiting case of the floating-gate NVSM, **single-electron memory cell** (Fig.4b)) **at room temperature** was first demonstrated by Yano et al.

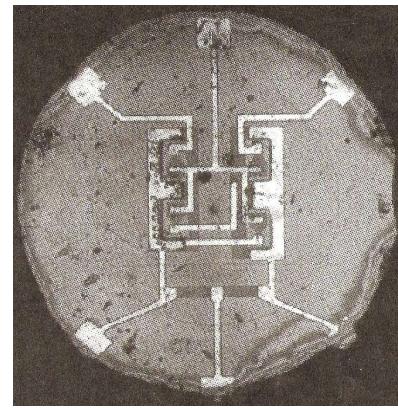
- **1970:** Boyle and Smith invented the **charge-coupled device (CCD)** which is used extensively in video cameras and in optical sensing applications.
- **1974:** The **resonant tunneling diode (RTD)** was first studied by Chang et al. RTD is the basis for most quantum-effect devices.
- **1980:** Minura et al. developed the **MODFET (modulation-doped field-effect transistor)**. With the proper selection of heterojunction materials, the MODFET is expected to be the fastest field-effect transistor.

## Key Semiconductor Technologies

- **1798:** The **lithography process** was invented. In this first process, the pattern, or image, was transferred from a stone plate (litho).
- **1918:** **Czochralski** developed a liquid-solid monocomponent growth technique. The **Czochralski crystal growth** is the process used to grow most of the crystals from which **silicon wafers** are produced.
- **1925:** Another growth technique was developed by **Bridgman**. The **Bridgman crystal growth** has been used extensively for the growth of gallium arsenide and related compound semiconductor crystals.
- **1952:** **Welker** noted that gallium arsenide and its related **III-V compounds** were semiconductors.

- **1952:** The **diffusion of impurity atoms** in semiconductors is important for device processing. The basic diffusion theory was considered by **Flick** in 1855. The idea of using **diffusion** techniques to alter the type of conductivity in silicon was disclosed in a patent by **Pfann**.
- **1957:** The ancient lithography process was applied to semiconductor-device fabrication by **Andrus**. He used **photosensitive etch-resistant polymers (photoresist)** for pattern transfer.  
Lithography is a key technology for the semiconductor industry. The continued growth of the industry has been the direct result of **lithographic photoresist technology**. Lithography is also a significant economic factor, currently representing over 35% of the integrated-circuit manufacturing cost.  
In the same year the **epitaxial growth process based on chemical vapor deposition technique** was developed by **Sheftal et al.**  
**Epitaxy**, derived from the Greek word epi, meaning on, and taxis, meaning arrangement, describes a technique of crystal growth to form a thin layer of semiconductor materials on the surface of a crystal that has a lattice structure identical to that of the crystal. This method is important for the improvement of device performance and the creation of novel device structures.

- **1959:** An integrated circuit (IC) was made by **Kilby**.
- Also, **Noyce** proposed the monolithic (single stone) IC by fabricating all devices in a single semiconductor substrate and connecting the devices by alluminum metallization. The alluminum interconnection lines were obtained by etching evaporated aluminum layer over the entire oxide surface using the lithographic technique.



**Fig.5**

- **1967:** The dynamic random access memory (DRAM) was invented by **Dennard**. The memory cell contains one MOSFET and one charge-storage capacitor. The MOSFET serves as a switch to charge or discharge the capacitor.

## Technology Trends

- The smallest line width or the minimum feature length of an integrated circuit has been reduced at a rate of about 13% per year. At that rate, the minimum feature length will shrink to about 50 nm in the year 2010. The cost per bit of memory chips has halved every 2 years for successive generations od DRAMs.

- The density of devices increases by a factor of 2 every 18 months.
- This is known as 'Moore's law'.

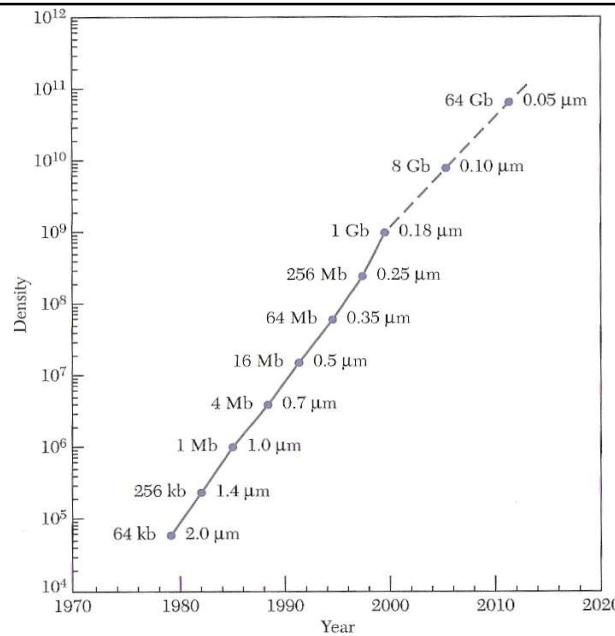
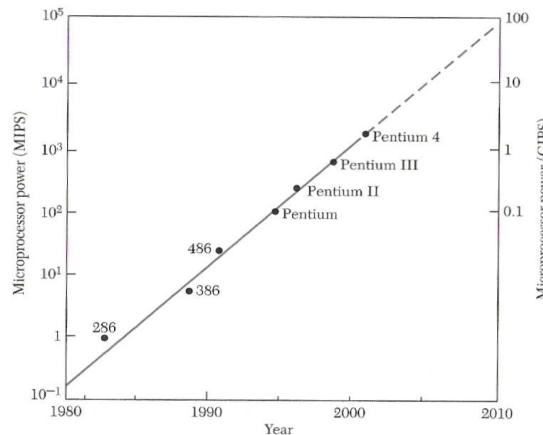


Fig 7 shows the exponential increase of the actual DRAM density versus the year of first production from 1978 to 2000.

- The computational power also increases by a factor of 2 every 18 months.



Exponential increase of the microprocessor computational power.

In a smartphone, there are about **one to two billion transistors**. They are responsible for many things such as turning the power on/off, processing information from sensors and controlling the screen display

### Important dates in the history of Semiconductor Physics:

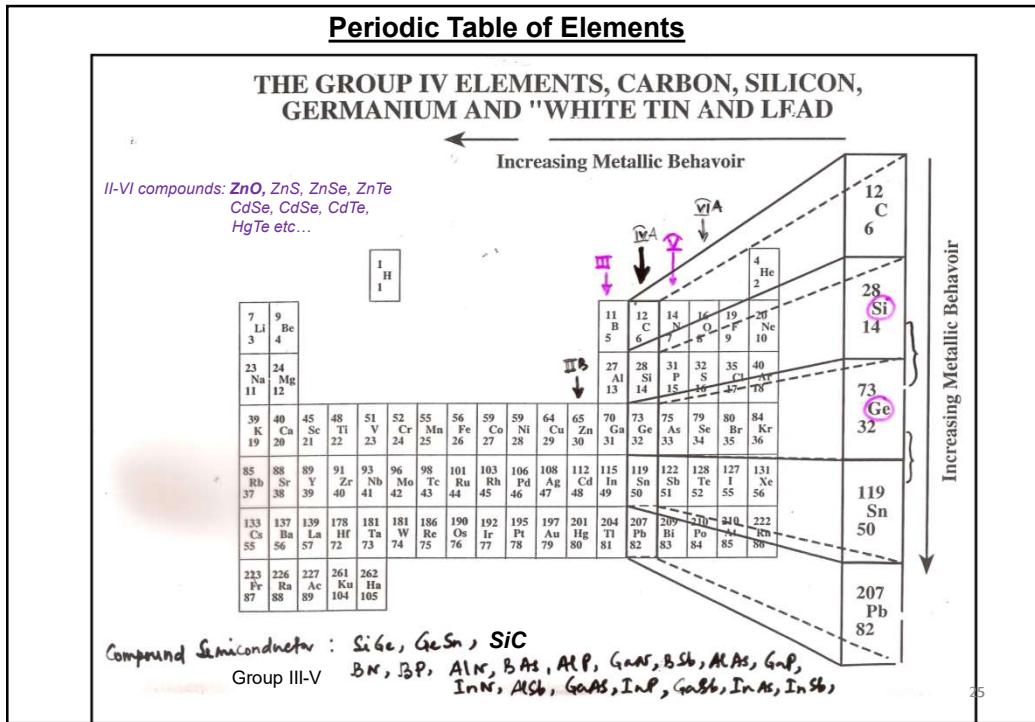
Year	Development
1897	Discovery of Hall effect, +ve Hall coefficient
1926	Bloch's theorem
1931	Wilson lays the foundation of the modern theory of semiconductors as insulators with narrow forbidden bands and introduced the idea of hole
1948	Discovery of the transistor by Bardeen & Brattain
1960	Appearance of planar technology
1982	World production of $3 \times 10^{13}$ binary units of active memory in the form of 64 kilo byte units alone
1990	Manufacture of DRAM of 4 MB per chip
1991	High definition TV camera with 2 MP CCD sensor
1992	Semiconductor component sales worldwide \$60 billion
1993	World production of transistors: $2 \times 10^{17}$
1995	Manufacture of 64-MB DRAM

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### Nobel Prizes for Semiconductor Research

- 1909 Carl Ferdinand Braun Wireless telegraphy, cat's whisker **rectifier**.
- 1956 John Bardeen, Walter Houser Brattain, William Shockley, **Transistor**.
- 1973 Leo Esaki **Tunnelling effect**.
- 1977 Sir Nevill Francis Mott, Philip Warren Anderson **Amorphous semiconductors**.
- 1985 Klaus von Klitzing **Quantum Hall effect**.
- 1998 Robert Laughlin, Horst Stormer, Daniel Tsui **Fractional quantum Hall effect**.
- 2000 Zhores Alferov, Herbert Kroemer **Semiconductor Heterostructures**, Jack Kilby **Integrated circuits**.
- 2009: Willard S. Boyle and George E. Smith “for the invention of an imaging semiconductor circuit – the **CCD sensor**”
- 2010: Andre Geim and Konstantin Nt**wo-dimensional material** ovoselov “for groundbreaking experiments regarding the graphene”
- 2014: Isamu Akasaki, Hiroshi Amano and Shuji Nakamura “for the invention of efficient **blue light-emitting diodes**”

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### Q.M. of the free electron moving in absence of any potential.

*Electrons inside the semiconductor can be regarded as “free” under proper condition.*

Schrodinger equation (time independent)

$$-\frac{\hbar^2}{2m_0} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

*General Solution:*

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{\pm ikr}, \quad \text{and} \quad E = \frac{\hbar^2 k^2}{2m}$$

$\frac{1}{\sqrt{V}}$  factor (normalization) comes because we wish to have one electron

$$\int_V d^3 r |\Psi(\mathbf{r})|^2 = 1$$

It is assumed that volume V is a cube of side L.

In classical mechanics,  $E = \frac{p^2}{2m}$ , p is a continuous variable.

In quantum mechanics,  $p=\hbar k$  due to wave nature of electrons, **k is discrete, not continuous.**

### Physical conditions

**Two kinds of boundary conditions** are imposed on wave functions

$\Psi \rightarrow 0$  at the boundary (as in the case of **Infininte Quantum well**)

So,  $\sin(k_x x) = 0$  for  $x=L$ .

Restricted k-values:

$k_x = \pi/L, 2\pi/L, 3\pi/L, \dots$ ,  $k \rightarrow$  positive values.

This is *standing wave solution* to quantum well describe the stationary electron confined in a fine region, such as.

**Periodic boundary condition for moving electrons,**  
 $\Psi(x+L, y, z) = \Psi(x, y, z) = \Psi(x-L, y, z)$  for a volume V.

The boundary condition impose certain restrictions in  $k$  of the wave function.

Energy of electron:

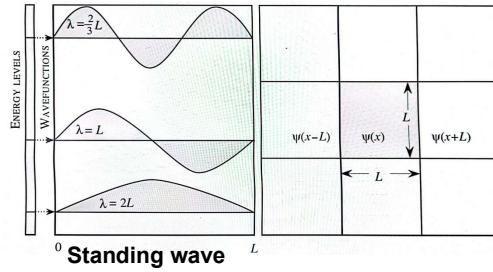
$$\frac{p^2}{2m_0} = \hbar^2 \frac{k^2}{2m_0}$$

Momentum

$$-i\hbar \frac{\partial}{\partial r} \rightarrow \hbar k$$

Velocity

$$\mathbf{v} = \hbar \frac{\mathbf{k}}{m_0}$$



Because of the boundary conditions, **allowed values of  $k$**  are ( $n_x, n_y, n_z$ , positive and negative both)

$$k_x = \frac{2\pi n_x}{L}, \frac{2\pi n_y}{L}, \dots$$

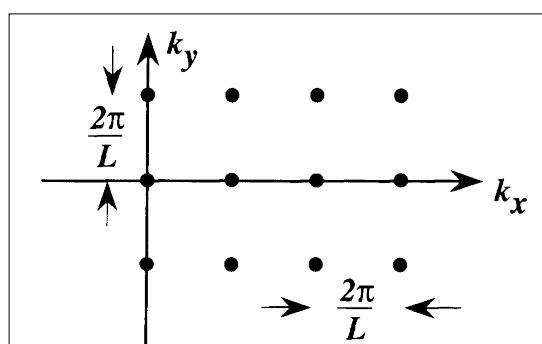
If  $L$  is large, allowed  $k$  spacing is small.

*Volume in  $k$ -space in 3D that each electronic state occupies*

$$\left(\frac{2\pi}{L}\right)^3 = 8\frac{\pi^3}{V}$$

No. of electronic states in volume  $\Omega$  of  $k$ -space

$$\frac{\Omega}{8\pi^3} = \frac{\Omega V}{8\pi^3}$$



This is used in the calculation of **density of states (DOS)**.

### Density of states (DOS)

The concept of density of states is extremely powerful, and important physical properties, such as optical absorption, electrical transport, etc., are intimately dependent upon this concept. **Density of states is the number of available electronic states per unit volume per unit energy around an energy E.** If we denote the density of states by  $N(E)$ , the number of states in a unit volume in an energy interval  $dE$  around an energy  $E$  is  $N(E)dE$ .

To calculate the density of states, we need to know the dimensionality of the system and the **energy vs. k relation** that the electrons obey.

If density of states is  $N(E)$ , **No. of states in dE interval =  $N(E) dE$** .

For calculation of DOS, we need to know the dimensionality and E-k relation. For free electron

$$E = \frac{k^2}{2m_0} \hbar^2$$

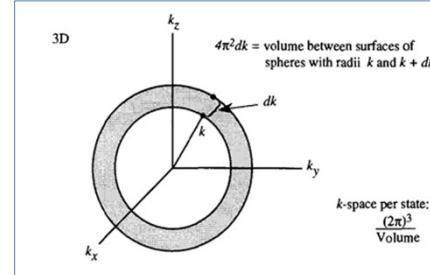
In the energy range  $E$  and  $E+dE$ , no. of electrons:

$$\frac{4\pi k^2}{8\pi^3} dk \cdot V = \frac{k^2}{2\pi^2} dk \cdot V$$

$$N(E) dE = \frac{k^2}{2\pi^2} dk$$

$$N(E) dE = \frac{m^{3/2}}{\pi^2 \hbar^3 \sqrt{2}} E^{1/2} dE$$

$$N(E) = \frac{m^{3/2}}{\pi^2 \hbar^3 \sqrt{2}} E^{1/2}$$



Using  $E = \frac{k^2}{2m_0} \hbar^2$

Accounting for spin of electron (Fermion) and effective mass, the DOS in 3-D is

$$N(E) = \frac{\sqrt{2}(m^*)^{3/2} E^{1/2}}{\pi^2 \hbar^3}$$

## Density of states in 2-D and 1-D:

Let us now consider a 2-D system, a concept that has become a reality with the use of **quantum wells**. Similar arguments tell that the density of states for a parabolic band is (including spin)

$$N(E) = \frac{m^*}{\pi \hbar^2}$$

Finally, in a 1-D system or a '**quantum wire**' the density of states is (including spin)

$$N(E) = \frac{\sqrt{2}m^*^{1/2}}{\pi \hbar} E^{-1/2}$$

We note that as the dimensionality changes, ***the energy dependence of the density of states also changes***. As shown in Fig. 3, for a 3-D system, we have a  **$E^{1/2}$  dependence**, for a 2-D system we have  **$E^0$**  (no energy dependence); and for a 1-D system we have an  **$E^{-1/2}$  dependence**.

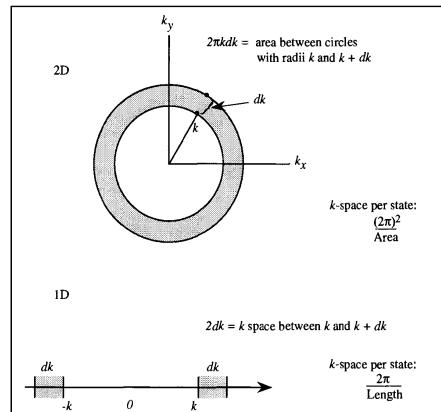


Fig. 2: Geometry used to calculate density of states in 3-, 2-, and 1-dimensions. By finding the &-space volume in an energy interval between  $E$  and  $E + dE$ , one can find out how many allowed states there

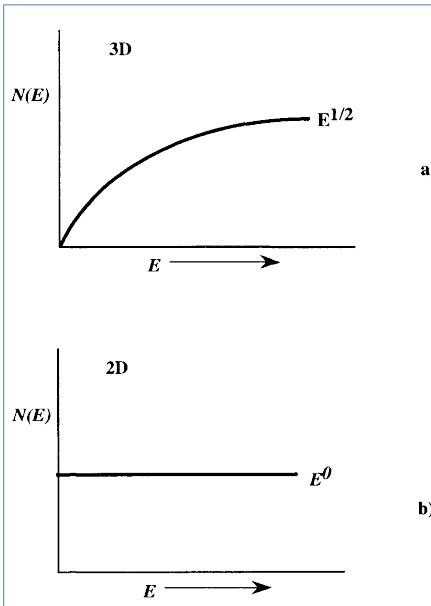


Fig. 3: Variation in the energy dependence of the density of states in (a) 3-dimensional, (b) 2-dimensional, and (c) 1-dimensional systems. The energy dependence of the density of states is determined by the dimensionality of the system. **This feature is exploited in advanced semiconductor devices.**

## Filling of Electronic States: Statistics

### How do the electrons distribute themselves among various allowed energy states?

Thermodynamics tells us that a system will be in equilibrium when its free energy is a minimum:

$$F = U - TS$$

↑      Entropy try to increase disorder.  
Internal energy would create order

In classical physics, all particles are *distinguishable* and hence can occupy same state. This leads to **Boltzmann distribution function** for occupancy.

But in QM, spin is important. A particular electronic state can be occupied by a single electron (**Fermion**). With +1/2 and -1/2 spins, two electrons can sit in a particular energy level. *Electrons with same spin are indistinguishable*.

Now we define a concept called **distribution function**  $f(E)$ :  $f(E)$  gives us the probability that states with energy  $E$  are occupied.

Classical or Maxwell-Boltzmann	$f(E) = \exp - \left( \frac{E - E_F}{k_B T} \right)$
Fermi-Dirac Distribution	$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{k_B T}}$
Bose-Einstein Distribution	$f(E) = \frac{1}{\exp \left( \frac{E}{k_B T} \right) - 1}$

$E_F$  is the Fermi energy and its value depends upon particle density).

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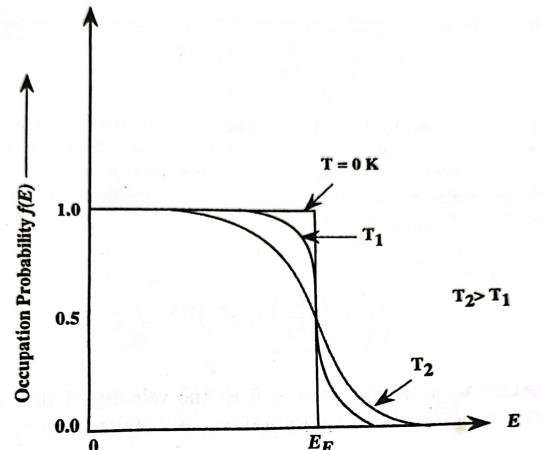
$$n = \int_0^{E_F} N(E) f(E) dE$$

For  $E < E_F$ ,  $f(E) \approx 1$ , at low  $T$

Otherwise,  $f(E) = 0$

$$n = \int_0^{E_F} N(E) dE$$

$$E_F = \frac{\hbar^2}{2m_0} (3\pi^2 n)^{2/3}$$



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## Periodicity of a crystal:

### Crystal structure --> lattice + basis

The various kinds of lattice structures possible in nature are described by the symmetry group that describes their properties. Rotation is one of the important symmetry groups. Lattices can be found which have a rotation symmetry. The rotation symmetries are denoted by 1, 2, 3, 4, and 6.

There are **14 types of lattices in 3D**. These lattice classes are defined by the relationships between the **primitive vectors  $a_1, a_2, a_3$  and the angles  $\alpha, \beta, \gamma$  between them**. Table 1 provides the basic properties of these three dimensional lattices.

We will focus on the **cubic lattice** which is the structure taken by all **semiconductors**.

**Table 1: The 14 Bravais lattices in 3-dimensional systems and their properties.**

System	Number of lattices	Restrictions on conventional cell axes and singles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

There are 3 kinds of cubic lattices: simple cubic (sc), body centered cubic (bcc), and face centered cubic (fcc).

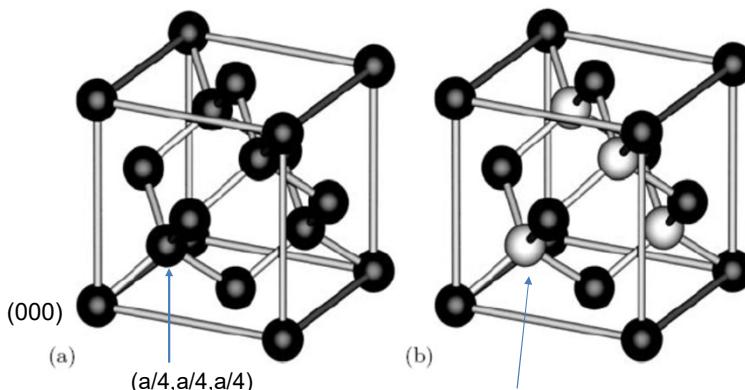
The fcc and bcc lattices are of great importance, since an enormous variety of solids crystallize in these forms with an atom (or ion) at each lattice site. Essentially all semiconductors of interest for electronics and optoelectronics have fcc structure.

### The Diamond and Zinc Blende Structures

Most semiconductors of interest for electronics and optoelectronics have an underlying fcc lattice. However, they have two atoms per basis. The coordinates of the two basis atoms are

$$(000) \text{ and } \left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$$

Since each atom lies on its own fcc lattice, such a two atom basis structure may be thought of as **two inter-penetrating fcc lattices**, one displaced from the other by a translation along a body diagonal direction  $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$ .



**Fig. 4:** (a) Diamond, (b) zinc blende crystal structure. The structure consists of the **interpenetrating fcc lattices**, one displaced from the other by a distance  $(a/4, a/4, a/4)$  along the **body diagonal**. The underlying Bravais lattice is fcc with a **two atom basis**. The positions of the two atoms is  $(000)$  and  $(a/4, a/4, a/4)$ .

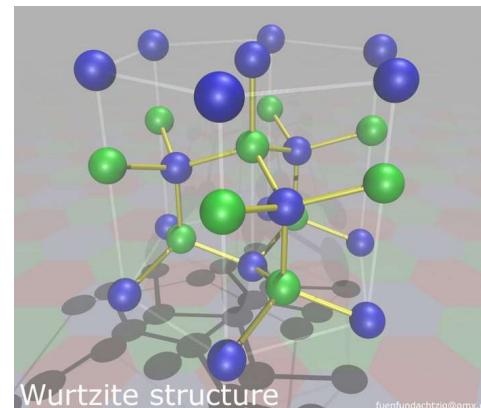
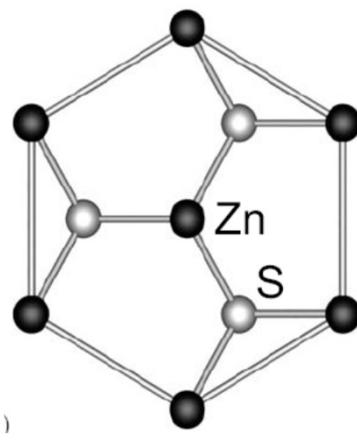
Figure 4 gives details of this important structure. If the two atoms of the basis are identical, the structure is called **diamond**. Semiconductors such as Si, Ge, C etc., fall in this category.

If the two atoms are different, the structure is called the **Zinc Blende structure**. Semiconductors such as GaAs, AlAs, CdS, etc., fall in this category. No. of atoms per unit cell is 8.

Semiconductors with diamond structure are often called **elemental semiconductors**, while the Zinc Blende semiconductors are called **compound semiconductors**. The compound semiconductors are also denoted by the position of the atoms in the periodic chart, e.g., GaAs, AlAs, InP are called **III-V (three-five) semiconductors**, while CdS, HgTe, CdTe, etc., are called **II-VI (two-six) semiconductors**.

Some semiconductors, such as ZnO, crystallizes in the wurtzite structure or hexagonal structure (Fig. 5).

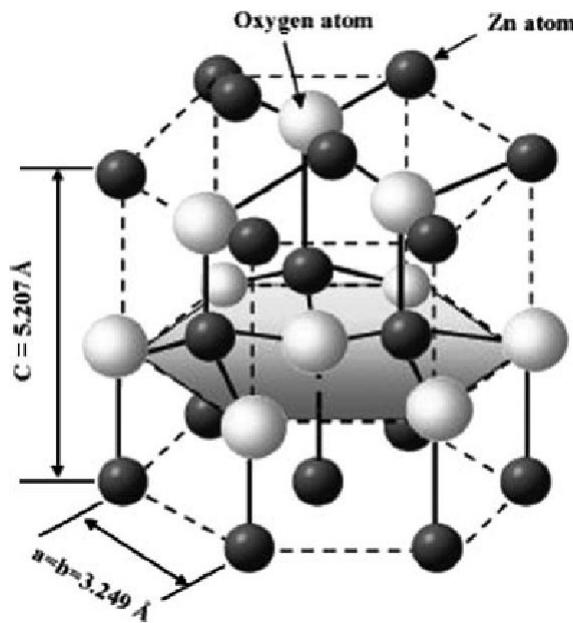
In a periodic structure, electrons do not scatter at all from ions. The effect of it is to alter apparent E-k relation of the electron, change the mass, introduce bandgap and even make electrons behave like positively charged particles.



Source: <http://commons.wikimedia.org/wiki/File:Wurtzite.jpg>

Fig. 5

ZnO



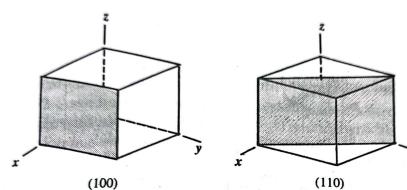
43

### Miller indices ( $h,k,l$ ):

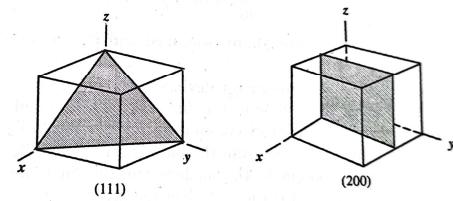
Notation to Denote Planes and points in a Lattice: Miller Indices

- Define x , y , z axis,
- Take the intercepts of planes along the axes in unit of lattice constant,
- take the reciprocal of the intercept and reduce them to smallest integers.

- The notation  $\{h, k, l\}$  – denotes a family of parallel planes/ equivalent planes.



- $\{100\}$ ,  $\{010\}$ ,  $\{001\}$  are equivalent planes.



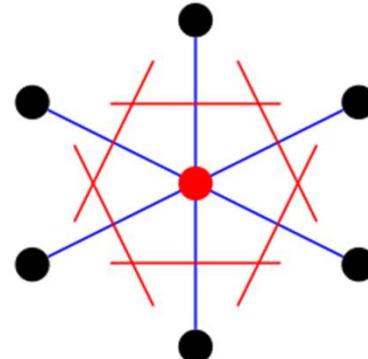
44

- To denote directions, we use the smallest set of integers having the same ratio as the direction cosines of the direction.
- In cubic system: Miller indices of a plane are the same as direction perpendicular to the plane.
- [ ] is for a set of parallel directions.
- < > is for a set of equivalent directions.

**Wigner Seitz cell:** The primitive cell of a reciprocal lattice can be represented by a Wigner-Seitz cell. It is defined in the reciprocal lattice-

- Draw lines to connect a given lattice point to all neighboring points.
- Draw bisecting lines or planes to the previous lines.

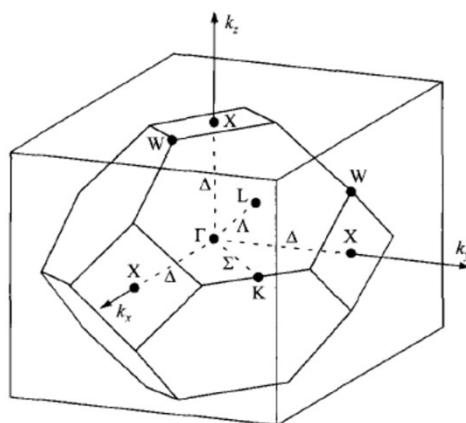
The volume enclosed within the bisection is called Wigner Seitz cell.



Wigner Seitz cell in 2D

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The Wigner-Seitz cell in the reciprocal lattice is called the first Brillouin zone.



Important high symmetry points

$$\Gamma \text{ point: } k_x = 0 = k_y = k_z$$

$$X \text{ point: } k_x = \frac{2\pi}{a}; k_y = k_z = 0$$

$$L \text{ point: } k_x = k_y = k_z = \frac{\pi}{a}$$

$a$  = lattice constant (cube edge)

Fig.6: Brillouin zones for fcc, diamond, and zinc blende lattices.

Reciprocal Lattice: Real space to k-space

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

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## Reciprocal lattice

- ❖ In physics, the reciprocal lattice represents the Fourier transform of another lattice. The direct lattice or real lattice is a periodic function in physical space, such as a crystal system (usually a Bravais lattice).
- ❖ The reciprocal lattice exists in the mathematical space of spatial frequencies, known as reciprocal space or  $k$  space, where  $k$  refers to the wavevector.
- ❖ In quantum physics, reciprocal space is closely related to momentum space according to the proportionality  $\mathbf{p} = \hbar \mathbf{k}$ , where  $\mathbf{p}$  is the momentum vector and  $\hbar$  is the reduced Planck constant.
- ❖ The reciprocal lattice of a reciprocal lattice is equivalent to the original direct lattice.
- ❖ The reciprocal lattice to an FCC lattice is the body-centered cubic (BCC) lattice, with a cube side of  $a$ .

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**Effective mass:**  $E = \frac{\hbar^2 k^2}{2m}$

for free electron,  $k^2$  determines the curvature of E-k curve. Curvature is found by double derivative of  $E$  w.r.t.  $k$ .  $1/m$  determines the curvature.

In real solid, the **E-k curvature determines the effective mass  $m^*$** , which is usually less than the free electron mass.

**Electrons in periodic potential:**

**Properties of electrons in a perfectly periodic crystal**

$$[-\frac{\hbar^2}{2m}\nabla^2 + \mathbf{U}(\mathbf{r})]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

$U(r)$  has same periodicity as crystal  $U(r)=U(r+R)$

$$\text{For } U(r)=0, \quad \Psi(r) = \frac{1}{\sqrt{V}} e^{ikr} \quad E = \frac{\hbar^2 k^2}{2m}$$

$$\text{For periodic } U(r) \quad \Psi_k(r) = e^{ikr} u_k(r)$$

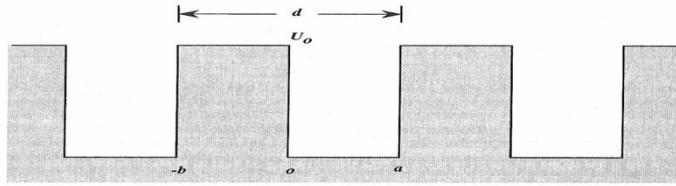
*In a periodic structure, electrons do not scatter at all from ions. The effect of it is to alter apparent E-k relation of the electron, change the mass, introduce bandgap and even make electrons behave like positively charged particles.*

**Bloch's theorem states that for a periodic potential,  $u_k$  has the same periodicity as the periodic potential.  $u_k(r) = u_k(r+R)$**

$$\Psi_k(r+R) = e^{ik(r+R)} u_k(r+R) = e^{ikr} \cdot u_k(r) e^{ikR} = e^{ikR} \Psi_k(r)$$

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### Kronig-Penny model for Band structure



$$U(x) = 0, \quad 0 \leq x \leq a$$

$$= u_0 \quad -b < x \leq 0$$

$$\Psi(x+d) = e^{i\theta} \Psi(x) \quad \text{where } \phi = k_x d$$

$$\Psi(x) = \begin{cases} Ae^{i\beta x} + Be^{-i\beta x}, & -b < x < 0 \\ De^{i\alpha x} + Fe^{-i\alpha x}, & 0 < x < a \end{cases} \quad \begin{aligned} \Psi(x) = & e^{i\phi} \{ A e^{i\beta(x-d)} + B e^{-i\beta(x-d)} \} & a < x < d \\ & D e^{i\alpha(x-d)} + F e^{-i\alpha(x-d)} & d < x < a + d \end{aligned}$$

Where,

$$\beta = \sqrt{\frac{2m_0(E-u_0)}{\hbar^2}} \quad \alpha = \sqrt{\frac{2m_0}{\hbar^2} E}$$

**Fig. 7:** The periodic potential to study the band structure in the Kronig-Penny model. The potential varies between 0 and  $u_0$  as shown and has a periodicity of  $d = a + b$ .

From continuity condition of wave function and its derivative at  $x=0$  and  $x=a$

$$We obtain, A + B = D + F$$

$$\beta(A - B) = \alpha(D - F)$$

$$\beta e^{i\theta} (A e^{i\beta b} - B e^{-i\beta b}) = \alpha (D e^{i\alpha a} - F e^{-i\alpha a})$$

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**Non-trivial solution** for the variables A, B, D, F are obtained **only if the determinant of the co-efficient vanishes**, which gives

$$\cos \phi = \cos a\alpha \cosh b\delta - \frac{\alpha^2 - \delta^2}{2\delta\alpha} \sin a\alpha \sin b\delta \quad , \quad \text{if } 0 < E < u_0$$

$$\cos \phi = \cos a\alpha \cos b\beta - \frac{\alpha^2 + \beta^2}{2\alpha\delta} \sin a\alpha \sin b\beta \quad , \quad \text{if } E > u_0$$

$$\text{where, } \delta = \sqrt{\frac{2m_0(u_0 - E)}{\hbar^2}}$$

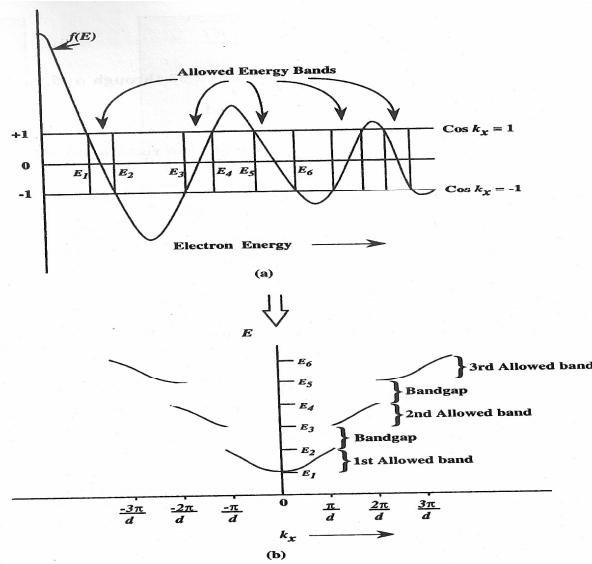
**Energy is physically allowed, only if  $-1 \leq \cos \phi \leq +1$**

If  $E < u_0$ , R.H.S. is denoted by  $f(E)$

$$f(E) = \cos(a \sqrt{\frac{2m_0 E}{\hbar^2}}) \cosh(b \sqrt{\frac{2m_0(u_0 - E)}{\hbar^2}}) + \frac{u_0}{\sqrt{E(u_0 - E)}} \sin(a \sqrt{\frac{2m_0 E}{\hbar^2}}) \sinh(b \sqrt{\frac{2m_0(u_0 - E)}{\hbar^2}})$$

The function must lie between -1 and +1, since it is equal to  $\cos \phi (= \cos k_x d)$ . We wish to find relationship between **E and  $\phi$  or E and  $k_x$** . Graphically one can see (Fig. 7(a)) that  $f(E)$  remains between  $\pm 1$  bounds only for certain region of energies. These are **allowed energies for the allowed bands and are separated by bandgaps**. One can obtain the bandstructure as shown in Fig. 8(b).

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**Fig. 8:** (a) The graphical solution to obtain the allowed energy levels. (b) The allowed and forbidden bands are plotted in the  $E$  vs.  $k$  relation using the results from fig. a. This  **$E$ - $k$  description is called band structure.**

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### Crystal momentum $\vec{p} = \hbar \vec{k}$

We know  $p = \hbar k$ , crystal momentum for free space.

$$\vec{k} = \frac{2\pi}{\lambda} \quad \text{crystal momentum inside the crystal.}$$

**Effect of the crystal is to modify the  $E$ - $k$  relationship.**

$\lambda$  wavelength is related to lattice spacing.

$k$  vectors are confined to **Brillouin zone**.

### Important high symmetry points

**$\Gamma$  point**  $k_x = k_y = k_z = 0$ , origin of the Brillouin zone.

**X point**  $k_x = \frac{2\pi}{a}$ ,  $k_y = k_z = 0$

**L point**  $k_x = k_y = k_z = \frac{\pi}{a}$

The value of  $k$  varies from 0 to some finite values determined by the lattice spacing. In the fcc lattice (for semiconductors), the  **$k$ -vector values are thus confined to a volume called the Brillouin zone**. This Brillouin zone for fcc lattice is shown in Fig. 6.

**The Brillouin zone looks like a truncated octahedron with the cube in the fcc structure.**

**From centre join eight corners and draw perpendicular bisectors to get the octahedron.**

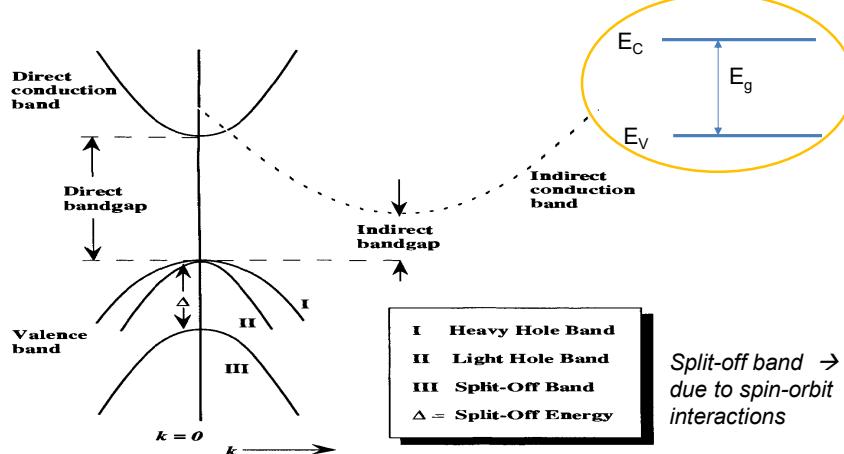
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## METALS, SEMICONDUCTORS AND INSULATORS

- ❖ When an **allowed band is completely filled with electrons**, the electrons in the band cannot conduct any current. This important concept is central to the special properties of **semiconductors**.
- ❖ When we have a material in which a **band is completely filled, while the next allowed band is separated in energy and empty**, the material has, in principle, infinite resistivity and is called an **insulator** or a **semiconductor**.
- ❖ The material in which a band is **only half full with electrons** has a very low resistivity and is called a **metal**.
- ❖ The band that is normally filled with electrons at 0 K in semiconductors is called the **valence band** while the upper unfilled band is called the **conduction band**.

➤ We have already discussed that the **solution of the Schrodinger equation leads to the band structure of the semiconductor**. The **top of the valence band of most semiconductors occurs at  $k=0$** , i.e., at effective momentum equal to zero. A typical band structure of a semiconductor near the top of the valence band is shown in Fig. 9

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**Fig. 9:** Schematic of the valence band, direct bandgap and indirect bandgap conduction bands. The conduction band of the **direct gap** semiconductor is shown in the solid line while the conduction band of the **indirect gap** semiconductor is shown in the dashed line. The valence band states are called holes.

Parabolic approximation is only valid near the symmetry points - in general the bands are not simple parabolas.

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Near the conduction band edges (occurring at  $k = k_0$ ) it is usually possible to represent the band structure by a simple relation of the form

$$E(k, k_o) = E(k_o) + \frac{\hbar^2}{2m_i^*} \sum_{i=x,y,z} \frac{(k_i - k_{oi})^2}{2m_i^*}$$

where the index  $i$  represents the x,y,z components of  $k$  or  $k_0$ . For direct bandgap materials  $k_0 = (0,0,0)$ .

If the band structure is isotropic as is the case for direct gap semiconductors, the relation becomes

$$E(k) = E_c + \frac{\hbar^2 k^2}{2m_i^*}$$

where  $E_c$  is the conduction band edge, and the band structure is a simple parabola with equal energy surfaces being the surfaces of a sphere.

For indirect materials like Si, the bottom of the conduction band occurs at six equivalent points:  $2\pi(0.85,0,0)/a$ ,  $2\pi(0,0.85,0)/a$ ,  $2\pi(0,0,0.85)/a$  and their inverses. The energy momentum relation has the form

$$E(k) = E_c + \frac{\hbar^2 k_l^2}{2m_l^*} + \frac{\hbar^2 k_t^2}{2m_t^*}$$

where  $k_l$  is the longitudinal part of  $k$  (i.e., parallel to the  $k$ -value at the bandedge) and  $k_t$  is the transverse part measured from the conduction bandedge  $k$ -value. The constant energy surface of the bandstructure is an ellipsoid.

Near the band edges, the electrons in semiconductors behave as if they have a mass  $m^*$  which is called the effective mass.

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For direct gap semiconductors, the effective mass of the electrons at the conduction band edge is given by the following approximate relation which results from detailed band structure calculations

$$\frac{1}{m^*} \cong \frac{1}{m_0} + \frac{2p_{cv}^2}{E_g}$$

where, for most semiconductors

$$\frac{p_{cv}^2}{m_0} \cong 20.0 \text{ eV}$$

where  $m_0$  is the free electron mass.

The conduction band effective mass thus decreases rapidly with decreasing bandgap.

Near the top of the valence band, in Fig. 9, there are two important curves. The heavier mass band is called the heavy hole band (I in Fig. 9). The second lighter band is called light hole band (II in Fig. 9).

The masses of the valence band electrons are usually much heavier than those in the conduction band and are also negative. The reason we call the valence band states "holes" will be discussed next.

In general, the effective mass is defined by the relation  $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}$

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### Concept of hole

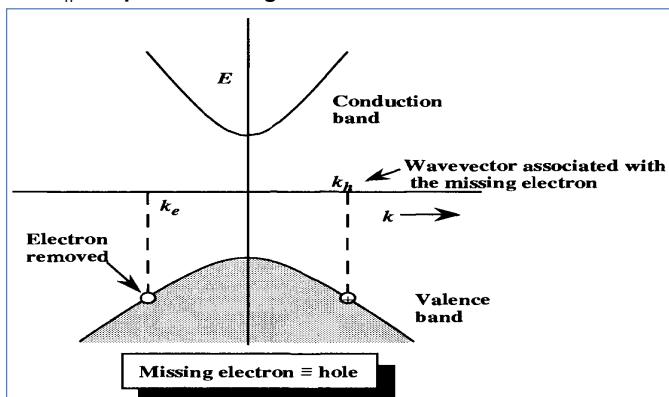
At 0K, valence band is full , conduction band is empty.

When all valence band states are filled,  $\sum k_i = 0 = \sum k_i + k_e$  where  $k_i \neq k_e$

**Missing states are called holes and wave vector of the system  $-k_e$  is attributed to it.**

If electron moves opposite to the field direction, unoccupied states or holes move in the field direction as if it has a mass  $m_h$  and positive charge

**Fig. 10:** Diagram illustrating the wave vector of the missing electron  $k_e$ . The wave vector of the system with the missing electron is  $-k_e$ , which is associated with the hole.



## BANDSTRUCTURES OF SOME IMPORTANT SEMICONDUCTORS

### Silicon

Silicon is the unchallenged material of choice for **electronic products**. The band structure of Si is shown in Fig. 11a. The **bandgap** is 1.1 eV with the **bottom of the conduction band occurring at  $k = (0.85*2\pi/a, 0, 0)$**  and the five other equivalent points, where  $a$  is the lattice constant (5.43 Å). The **band structure near the conduction band minima** is ( $k$  is measured from the band edge value)

$$E(k) = \frac{\hbar^2 k_i^2}{2m_i^*} + \frac{\hbar^2 k_t^2}{2m_t^*}$$

where  $m_i^* = 0.98 m_0$  and  $m_t^* = 0.19 m_0$ , and gives **ellipsoid constant energy surfaces** (Fig. 11b).

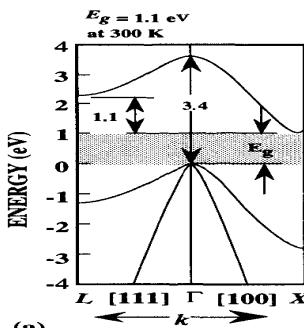


Fig. 11 (a)

**Gamma point :  $k = (0,0,0)$**   
**X point :  $k = \frac{2\pi}{a} (1,0,0)$**   
**L point :  $k = \frac{\pi}{a} (1,1,1)$**

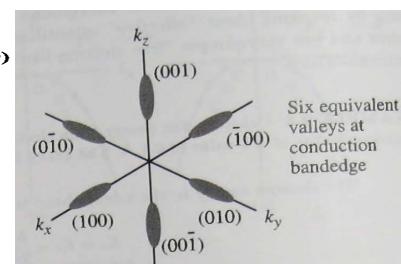
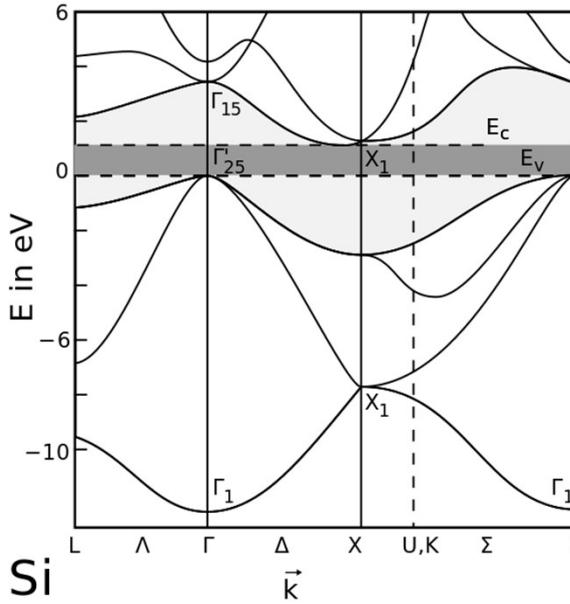


Fig. 11(b)

## Schematics of calculated band structure of crystalline Si

Physical Review B 10, 5095-5107(1974)



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Being an **indirect material**, Si has very poor optical properties and cannot be used to make **lasers**. The reason for this is the need for "vertical k" transitions for optical processes due to momentum conservations. The hole transport properties of Si are also quite poor, since the hole masses are quite large. However, for electronic devices, silicon is the material of choice because of its highly reliable processing technology.

### GaAs (Gallium Arsenide)

The band structure of GaAs is shown in Fig. 12. The bandgap is direct which is the chief attraction of GaAs. The **direct bandgap** ensures **excellent optical properties** of GaAs as well as **superior electron transport** in the conduction band. The band edge **E vs k relation is quite isotropic** leading to spherical equal energy surfaces. The bandstructure can be represented by the relation

$$E = \frac{\hbar^2 k^2}{2m^*}$$

with  $m^* = 0.067 m_o$ . A better relationship is the **non-parabolic**

$$\frac{\hbar^2 k^2}{2m^*} = E(1 + \alpha E)$$

with  $\alpha = 0.67 \text{ eV}^{-1}$ . The values of the hole masses are  $m_{hh}^* = 0.45 m_o$ ,  $m_{lh}^* = 0.1 m_o$ .

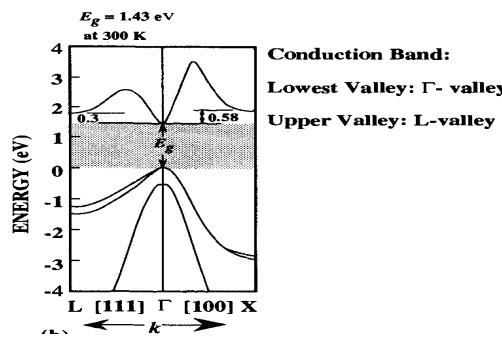
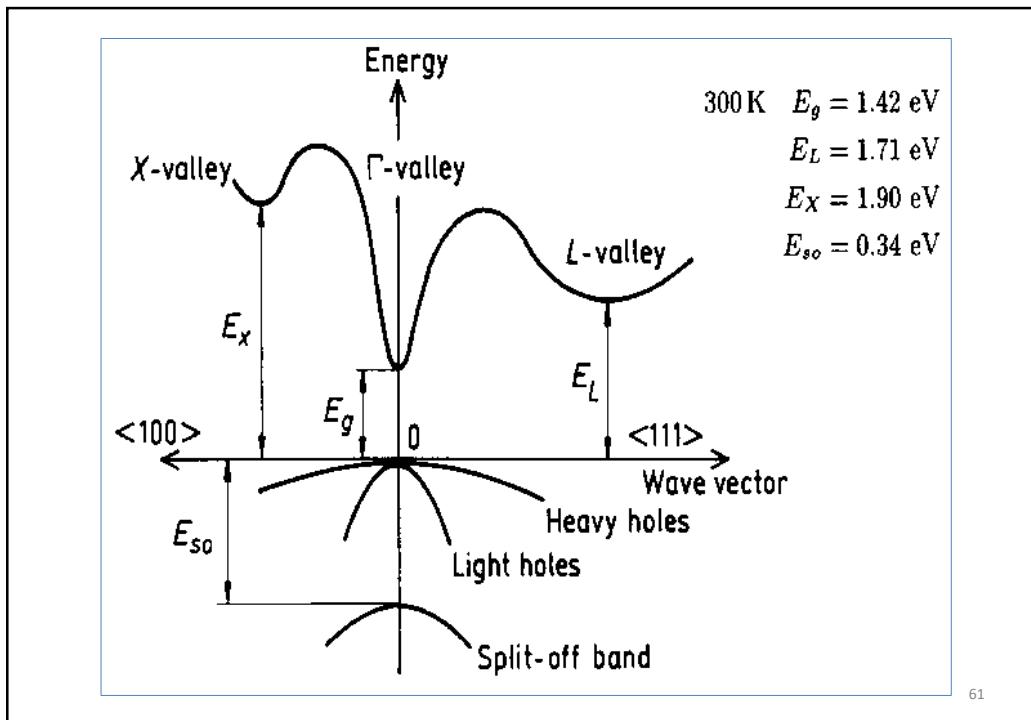
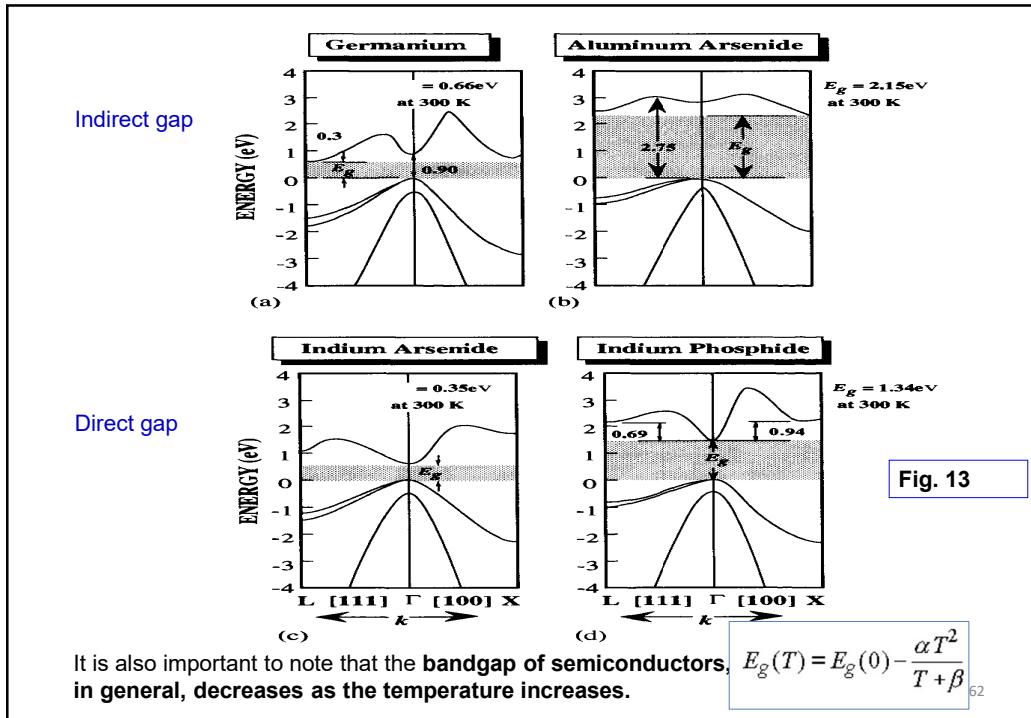


Fig. 12

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## Band structure modification : By Alloying, Heterostructure, Strain

### (i) Alloying of two or more semiconductors

Vegard's law : (i)  $a_{\text{alloy}} = x a_A + (1-x) a_B$

**Band gap of the alloy:**  $E_g^{\text{alloy}} = x E_g^A + (1-x) E_g^B$

Due to disorder, there is a **bowing effect**:  $E_g^{\text{alloy}} = a + bx + cx^2$  C is the bowing parameter.

### (ii) Hetero structures

Epitaxial technique of crystal growth.

Using epitaxial technique to grow sequence of semiconductor layer with different band gaps.

An important example is the GaAs and the  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  system, which have a very good match of their lattice constants.

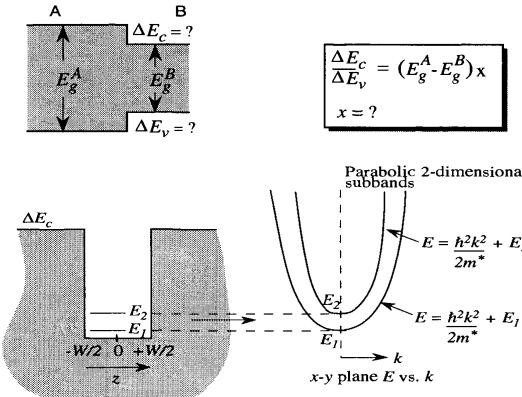


Fig. 14

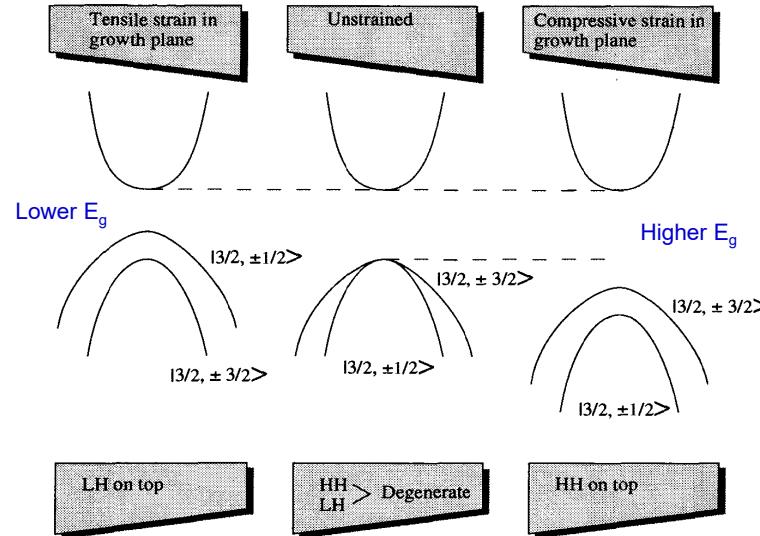
An extremely important parameter in the **quantum well** problem is the **band-edge discontinuity** produced when two semiconductors are brought together. As shown in Fig. 14a, a part of the bandgap discontinuity ( $E_g^A - E_g^B$ ) of two semiconductors A and B would appear in the conduction band and a part would appear in the valence band.

Once the band discontinuity is known, the band structure of a quantum well structure can be calculated. The simplest way to do this is to use the effective mass theory in which the electron in each region of the structure is represented by its effective mass.

**The effect of the quantum well is to impose a background confining potential.**

**Due to confinement of electrons, there is sub-band formation** (see Fig. 14b). **The effective band-gap changes.** These sub-bands have important consequences for optical and transport properties of hetero-structures.

### (iii) Band structure modification by Strain:



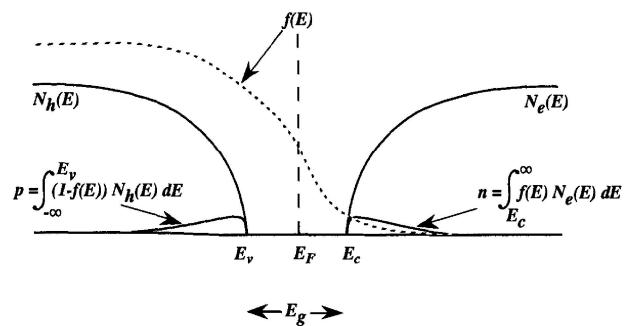
**Fig. 15:** The consequence of pseudomorphic strain on the band edges of a direct bandgap semiconductor. The valence band degeneracy at  $k = 0$  is lifted as the HH and LH states are split as shown.

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### INTRINSIC CARRIER CONCENTRATION

The intrinsic carrier concentration depends upon the bandgap and temperature and the details of the band edge masses. We will assume that the band edge density of states for electrons and holes originate from parabolic E-k relationships. The conduction and valence band density of states are shown in Fig. 16 along with the position of a Fermi level.

**Fig.16:** A schematic of the density of states of the conduction and valence band.



The concentration of electrons in the conduction band is

$$n = \int_{E_c}^{\infty} N_e(E) f(E) dE$$

$$n = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \int_{E_c}^{\infty} \frac{(E - E_c)^{1/2} dE}{\exp(\frac{E - E_F}{k_B T}) + 1}$$

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$$\begin{aligned} n &= \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \exp \left( \frac{E_F}{k_B T} \right) \int_{E_c}^{\infty} (E - E_c)^{1/2} \exp(-E/k_B T) dE \\ &= 2 \left( \frac{m_e^* k_B T}{2\pi\hbar^2} \right)^{3/2} \exp[(E_F - E_c)/k_B T] = N_c \exp[(E_F - E_c)/k_B T] \end{aligned}$$

where

$$N_c = 2 \left( \frac{m_e^* k_B T}{2\pi\hbar^2} \right)^{3/2}$$

$$\begin{aligned} N_c &= 2 \left( \frac{m_{dos}^* k_B T}{2\pi\hbar^2} \right)^{3/2} \\ &= 2 \left( \frac{1.06 \times 0.91 \times 10^{-30} \text{ (kg)} \times 4.16 \times 10^{-21} \text{ (J)}}{2 \times 3.1416 \times (1.05 \times 10^{-34} \text{ (Js)})^2} \right)^{3/2} \text{ m}^{-3} \\ &= 2.78 \times 10^{25} \text{ m}^{-3} = 2.78 \times 10^{19} \text{ cm}^{-3} \end{aligned}$$

$N_c$  is known as the effective density of states at the conduction band-edge.

The carrier concentration is known when  $E_F$  is calculated. To find the intrinsic carrier concentration, this requires finding the **hole concentration p as well**.

$$\begin{aligned} p &= 2 \left( \frac{m_h^* k_B T}{2\pi\hbar^2} \right)^{3/2} \exp [-(E_v - E_F)/k_B T] \\ &= N_v \exp [-(E_v - E_F)/k_B T] \end{aligned}$$

where  $N_v$  is the effective density of states for the valence bandedge.

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In intrinsic semiconductors, the electron concentration is equal to the hole concentration since each electron in the conduction band leaves a hole in the valence band. If we multiply the electron and hole concentrations, we get

$$np = 4 \left( \frac{k_B T}{2\pi\hbar^2} \right)^3 (m_e^* m_h^*)^{3/2} \exp(-E_g/k_B T)$$

and since for the intrinsic case  $n = n_i = p = p_i$ , we have from the square root of the equation above

$$n_i = p_i = 2 \left( \frac{k_B T}{2\pi\hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} \exp[-(E_c + E_v)/2k_B T]$$

If we set  $n = p$ , we also obtain the Fermi level position measured from the valence band edge

$$\exp(2E_{Fi}/k_B T) = (m_h^*/m_e^*)^{3/2} \exp(E_g/k_B T)$$

$$E_{Fi} = \frac{E_c + E_v}{2} + \frac{3}{4} k_B T \ln(m_h^*/m_e^*)$$

Thus the **Fermi level of an intrinsic material lies close to the midgap**.

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Note that the **carrier concentration increases exponentially as the bandgap decreases** and has a strong temperature dependence.

We note that the product  $np$  calculated above is independent of the Fermi level  $E_F$ . This is an expression of the law of mass action. This result is valid not only for the intrinsic case but also when we have dopants.

At room temperature, the  $np$  product is  $2.25 \times 10^{20} \text{ cm}^{-6}$ ,  $5.76 \times 10^{26} \text{ cm}^{-6}$  and  $3.24 \times 10^{12} \text{ cm}^{-6}$  for Si, Ge, and GaAs, respectively. The corresponding intrinsic carrier densities are  $1.5 \times 10^{10} \text{ cm}^{-3}$ ,  $2.4 \times 10^{13} \text{ cm}^{-3}$  and  $1.8 \times 10^6 \text{ cm}^{-3}$ , respectively. Temperature dependence: Fig. 17

- It is quite clear that pure semiconductors have a very low concentration of carriers that can conduct current. One must compare the room temperature concentrations of  $\sim 10^{11} \text{ cm}^{-3}$  to the carrier concentrations of  $\sim 10^{21} \text{ cm}^{-3}$  in metals. Indeed, pure semiconductors would have little use by themselves.
- Doping of impurities is essential to increase the carrier concentration in semiconductors. The dopants are chosen from the periodic table so that they either have an extra electron in their outer shell compared to the host semiconductor, or have one less electron. The resulting dopant is called a donor or acceptor.

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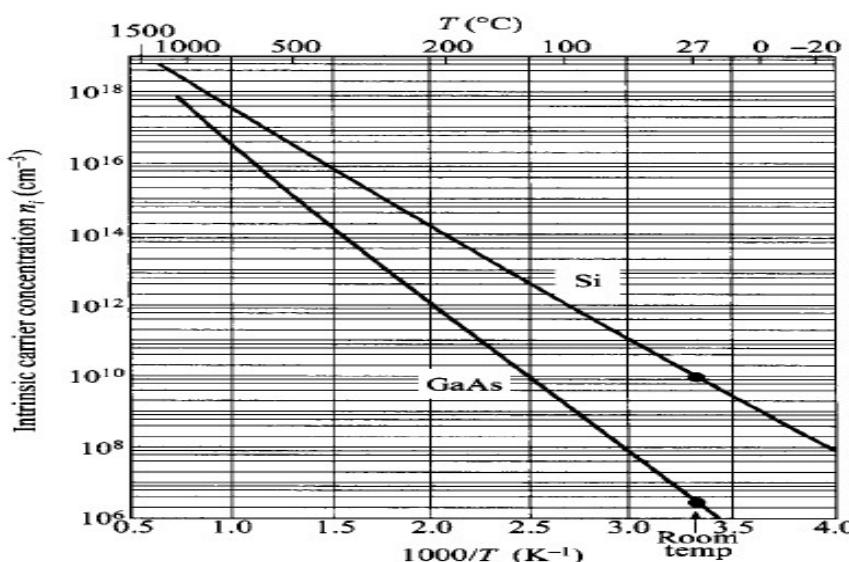
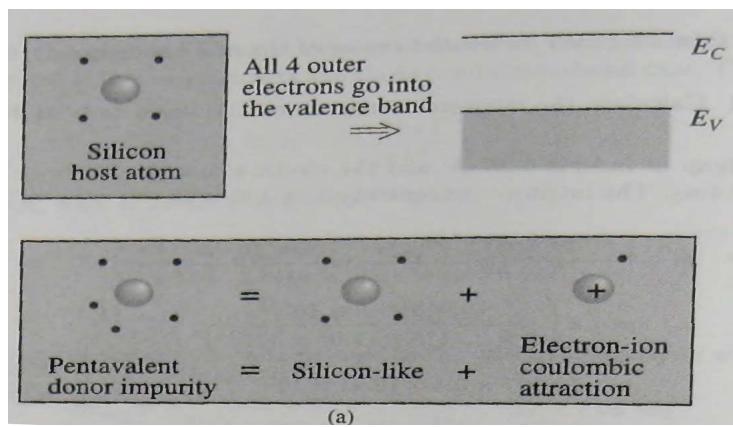


Fig. 17: Intrinsic carrier concentrations of Si and GaAs as a function of reciprocal temperature.

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**Fig. 18:** Schematic for understanding donors in semiconductors

- The **donor atom is treated as a shallow defect and the electron-donor interaction is represented by a Coulombic potential.**
- The problem is solved by a **simple analogy to the hydrogen atom problem.**
- The **donor produces a shallow level whose energy is simply given by the hydrogen atom problem in quantum mechanics**, except that the mass of the electron is replaced by the **effective mass** at the conduction bandedge:

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$$\begin{aligned}
 E_d &= E_c - \frac{e^* m_e^*}{2(4\pi\epsilon)^2 \hbar^2} \\
 &= E_c - 13.6 \left( \frac{m^*}{m_0} \right) \left( \frac{\epsilon_0}{\epsilon} \right)^2 eV
 \end{aligned}$$

0.025 eV for Si  
0.007 eV for GaAs

donor energy levels depend only upon the host crystal (through  $\epsilon$  and  $m^*$ ) and not on the nature of the dopant.

**Conductivity effective mass ( $m^*$ ):** response of electrons to external potentials/field.

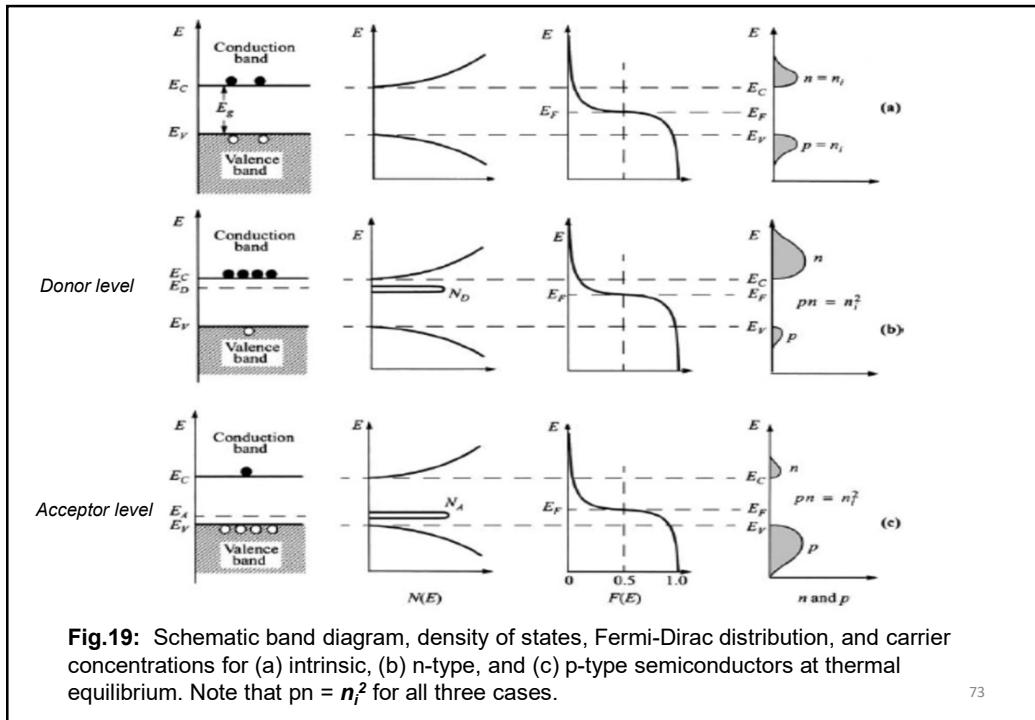
This mass is used for donor energies as well as for charge transport in an electric field.

For **direct bandgap materials like GaAs, this is simply the effective mass.**

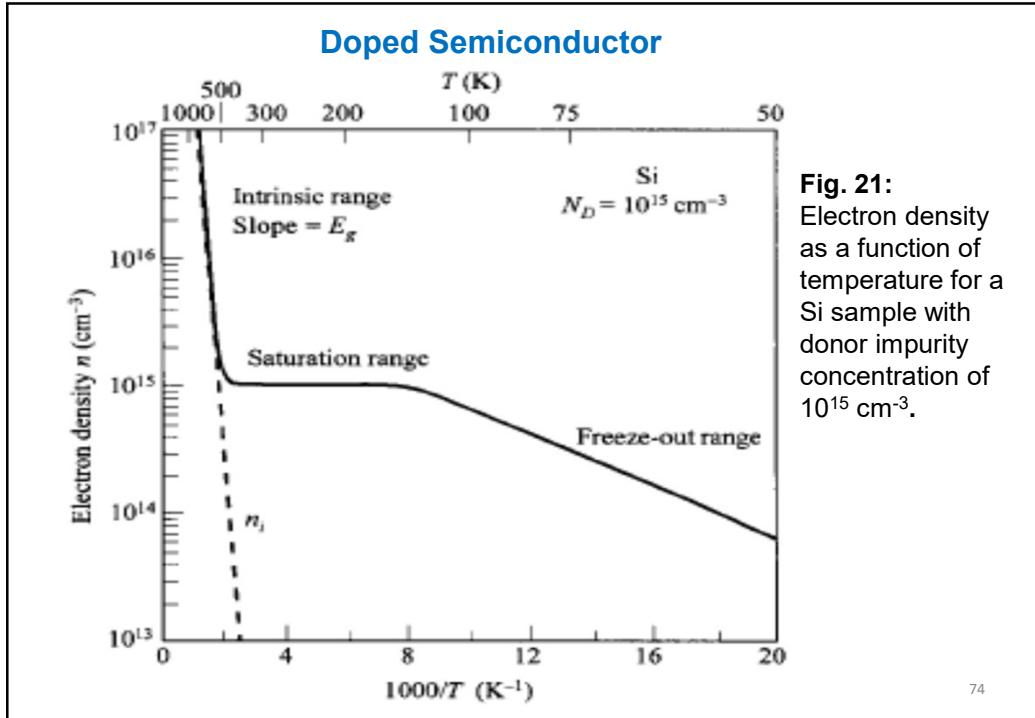
For materials like **Si the conductivity mass is**

$$m_\sigma^* = 3 \left( \frac{2}{m_t^*} + \frac{1}{m_\ell^*} \right)^{-1}$$

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### Extrinsic Carrier Density

In the lowest energy state of the donor atom, the extra electron of the donor is trapped at the donor site and occupies the donor level  $E_d$ . Such an electron cannot carry any current and is not useful for changing the electronic properties of the semiconductor. At very low temperatures, the donor electrons are, indeed, tied to the donor sites and this effect is called carrier freeze out. At higher temperatures, however, the donor electron is "ionized" and resides in the conduction band as a free electron. Such electrons can, of course, carry current and modify the electronic properties of the semiconductor. The ionized donor atom is positively charged.

Because of the doping (Nd is the donor density, Na is the acceptor density), we no longer have the equality between electrons and holes, i.e.,

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$$n - p = \Delta n \neq 0$$

However, the law of mass action still holds (the value of the product changes only at high doping levels)

$$np = \text{constant} = n_i^2$$

If we eliminate p in these equations we get, after solving a quadratic equation

$$n = \frac{1}{2}\Delta n + \frac{1}{2}(\Delta n^2 + 4n_i^2)^{1/2}$$

Similarly, we have for the holes

$$p = -\frac{1}{2}\Delta n + \frac{1}{2}(\Delta n^2 + 4n_i^2)^{1/2}$$

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Using approximation the distribution function can be replaced by Boltzmann like function

$$f(E) = \exp(-(E - E_F)/k_B T)$$

And we get

$$\frac{n}{n_i} = e^{(E_F - E_{F,i})/k_B T} \quad \text{for electron}$$

$$\frac{p}{n_i} = e^{-(E_F - E_{F,i})/k_B T} \quad \text{for hole}$$

Where  $E_F$  is the fermi level and we get

$$\frac{n-p}{n_i} = \frac{\Delta n}{n_i} = 2 \sinh \left( \frac{(E_F - E_{F,i})}{k_B T} \right)$$

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And the carrier density is

$$n = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \int_{E_c}^{\infty} \frac{(E - E_c)^{1/2} dE}{\exp \left( \frac{E - E_F}{k_B T} \right) + 1}$$

Where,

$$\eta = \frac{E - E_c}{k_B T}; \eta_F = \frac{E_F - E_c}{k_B T}$$

$$n = \frac{1}{2\pi^2} \left( \frac{2m^* k_B T}{\hbar^2} \right)^{3/2} \int_0^{\infty} \frac{\eta^{1/2} d\eta}{\exp(\eta - \eta_F) + 1}$$

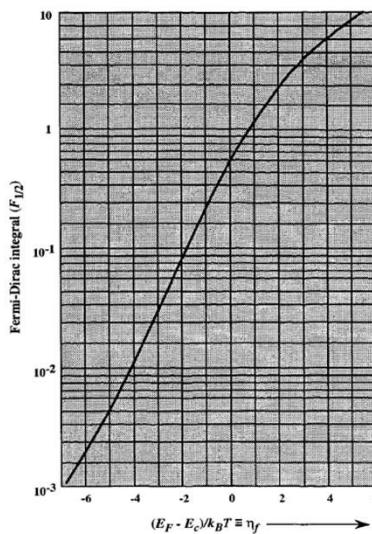
$n = \frac{2}{\sqrt{\pi}} N_c * \text{Fermi integral}$

A useful expression for the relation between carrier concentration and Fermi level is Joyce-Dixon approximation.

$$E_F = E_c + k_B T \left[ \ln \frac{n}{N_c} + \frac{1}{\sqrt{8}} \frac{n}{N_c} \right] = E_v - k_B T \left[ \ln \frac{p}{N_v} + \frac{1}{\sqrt{8}} \frac{p}{N_v} \right]$$

*This relation can be used to obtain the Fermi level if n is specified.*

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$$n = \frac{2}{\sqrt{\pi}} N_c * \text{Fermi integral}$$

Figure 3.17: A plot of the Fermi-Dirac integral as a function of Fermi level. The graph can be used to calculate an accurate value of the electron or hole densities for a given position of the Fermi level.

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**EXAMPLE 3.6** Assume that the Fermi level in silicon coincides with the conduction band edge at 300 K. Calculate the electron carrier concentration using the Boltzmann approximation, the Joyce-Dixon approximation, and the Fermi-Dirac integral.

In the Boltzmann approximation, the carrier density is simply

$$n = N_c = 2.78 \times 10^{19} \text{ cm}^{-3}$$

According to the Joyce-Dixon approximation, the carrier density is obtained from the solution of the equation

$$E_F = 0 = k_B T \left[ \ln \frac{n}{N_c} + \frac{1}{\sqrt{8} N_c} \right]$$

This gives

$$\frac{n}{N_c} = 0.76 \text{ or } n = 2.11 \times 10^{19} \text{ cm}^{-3}$$

From the Fermi-Dirac integral we see that at  $\eta_F = 0$ ,  $F_{1/2}(0) \approx 0.65$ .

$$n = \frac{2}{\sqrt{\pi}} N_c F_{1/2}(0) = 0.74 N_c$$

We see that the Joyce-Dixon result gives a very close match with the exact calculation using the Fermi-Dirac integral. However, in this case the Boltzmann approximation gives a higher charge density.

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**Degenerate Semiconductors:** High doping density, probability of band-edge electronic levels are occupied by electrons/ holes is close to 1.

Bandgap narrowing at high doping :  $\Delta E_g \cong 22.5 \left( \frac{N_d}{10^{18}} \frac{300}{T(K)} \right)^{1/2}$  meV. At high doping level, it overestimates the bandgap narrowing.

### Modulation Doping

Avoid Impurity electron scattering. Controllable free carrier density without scattering. Hetero structure with high band gap region doped. (GaAs/AlGaAs).

$$\text{DOS in QW}, \quad N_{2D}(E) = \frac{m^*}{\pi \hbar^2}$$

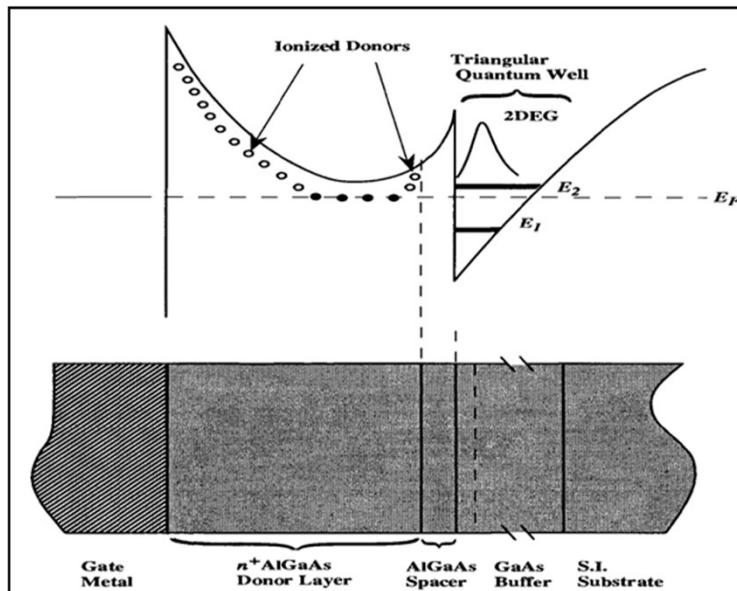
Fermi level is measured from bottom of subband  $E_1$ .

$$n_{2D} = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{E_F - E_1}{k_B T} \right) \right]$$

$$E_F - E_1 = k_B T \ln \left[ \exp \left( \frac{n_{2D} \pi \hbar^2}{m^* k_B T} \right) - 1 \right]$$

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**Modulation doped heterostructure. Electrons are transferred to the narrow gap region where one has 2D electron gas.**



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### **Doping Techniques:**

- 1. Epitaxial techniques** : Where dopant is introduced during growth.
- 2. Ion-implantation** : High energy dopant ions are implanted into semiconductors.
- 3. Diffusion:** When a lump of the dopant material is placed on the semiconductor & is annealed causing a diffusion of the dopant atoms into semiconductor.

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