Energy Bands and Charge Carriers in Semiconductors

We are interested in

(1) How to make <u>different charge distribution</u>: use doping, n+ and p+ type regions in p and n type substrate

(2) How to make carriers (positive and negative charges; holes and electrons) move (transport) from one location to the other <u>in a controlled way</u> (by applying bias – gate bias to form a conducting channel, drain bias to let majority carriers move; by removing bias – energy barrier to block the carrier flow)

Let's try to understand energy bands, doping, Fermi level, etc., which are fundamental concepts of above issues in solid state electronic devices

Bands

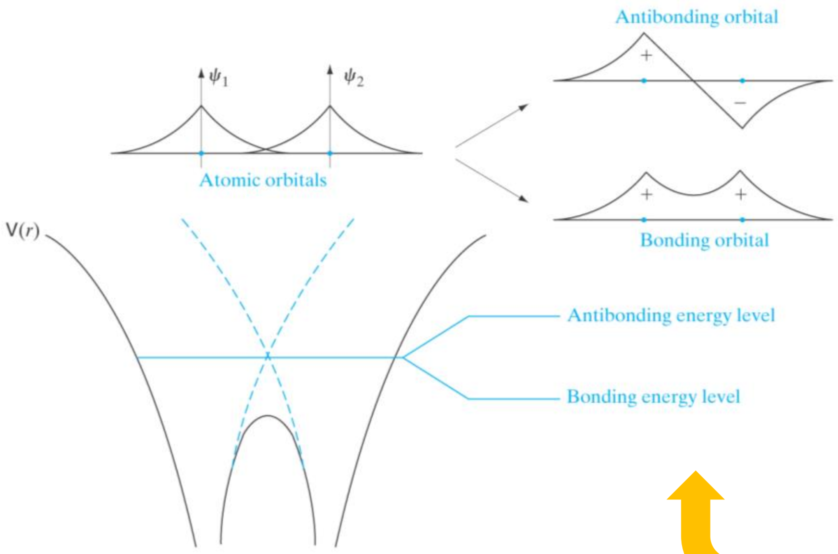
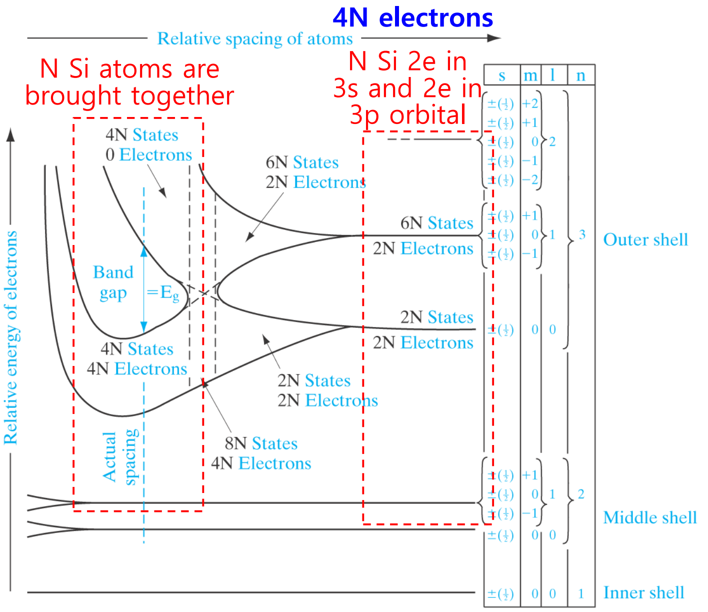


Figure 3.2

- Figure 3.2 (left) shows schematic coulombic potential wells of two atoms.
- The composite two-electron wave functions are linear combination of individual atomic orbitals : anti-symmetric combination is anti-bonding, and symmetric combination is bonding orbital.
- Bonding orbital has higher value of wave function (more electron) in between the two nuclei.
- Since electrons in between are attracted by two nuclei, the potential energy of bonding is lower than anti-bonding.

- The number of distinct energy levels (split by bonding and antibonding) depends on the number of atoms brought together.
- The lowest and highest energy level correspond to entire bonding and entire anti-bonding, respectively.
- In a solid, many atoms are brought together, so that the split energy levels from essentially continuous bands of energy.
- In silicon, **the upper band (conduction band) contains 4N state (no electron at O K) and lower band (valence band) contains 4N state (4N electrons at O K).** There is a forbidden state, called a band gap, between the two bands.



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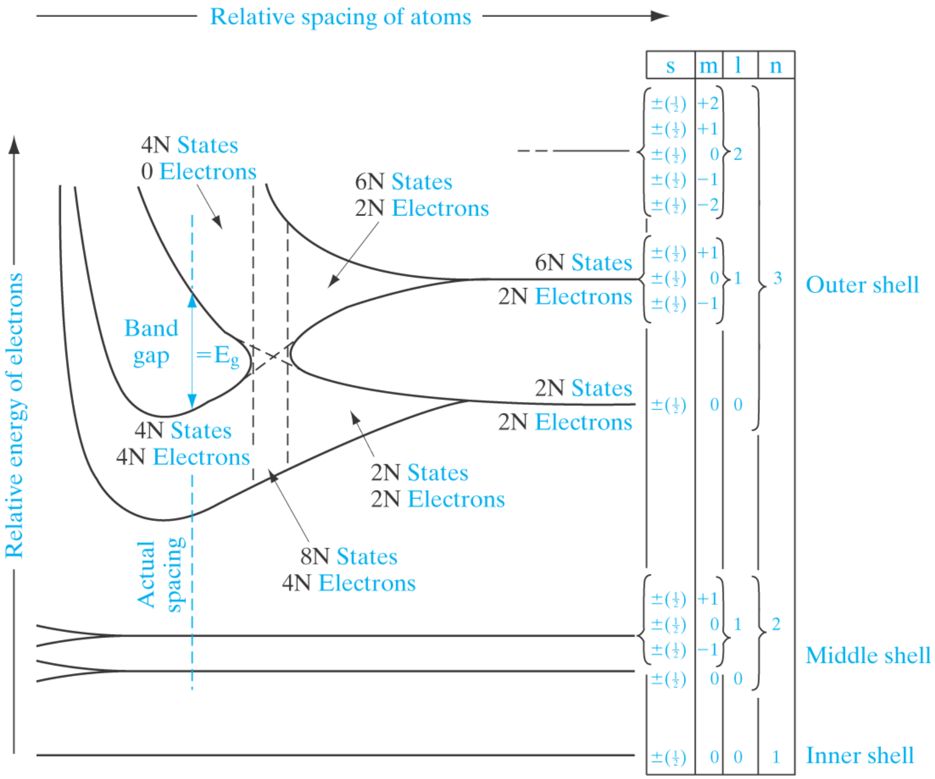
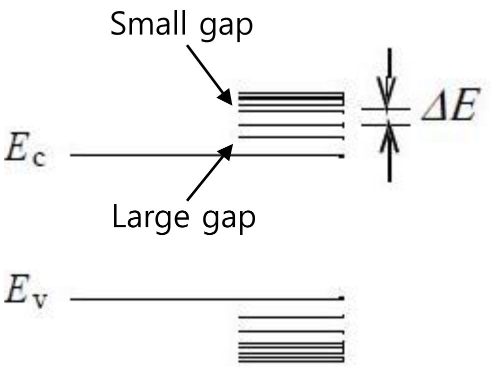
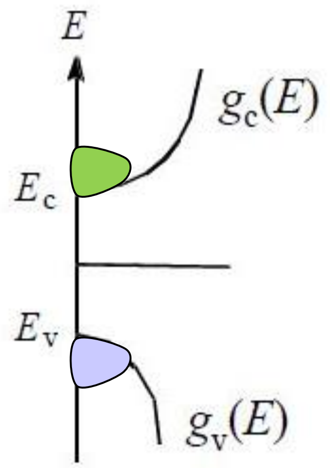
Bands: Density of States







$$g_c(E)=\frac{m_n^*\sqrt{2m_n^*(E-E_c)}}{\pi^2\hbar^3} \quad E\geq E_c$$

$$g_v(E)=\frac{m_p^*\sqrt{2m_p^*(E_v-E)}}{\pi^2\hbar^3} \quad E\leq E_v$$

Higher density of state as the energy state is far from the band edge.

- The density of states (g(E)) describes the <u>number of states per interval of energy at each energy level that are available to be occupied by electrons</u>.
- i.e. g(E)dE = number of states/cm^3 in the energy range between E and E+dE.

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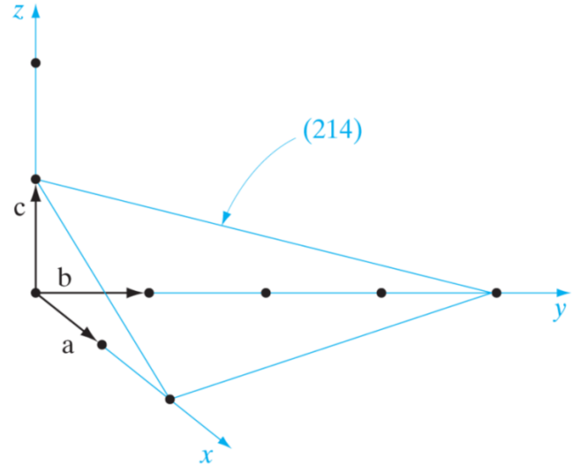
Crystal Structure: Planes and Directions

- When we discuss about single crystal materials, it is very useful to use planes and directions of the lattice, such as [hkl], where h, k, l are integers.
- For example, [100] surface or [111] surface of single crystal silicon wafer have different electrical and chemical properties. [100] surface has higher electron mobility and higher etching rate than [111] surface.
- The three integers describing a particular plane are found in the following way:
  - (1) Find the intercepts of the plane with the crystal axes. Then express these intercepts by using basis vectors multiplied with integers.
  - (2) Take the reciprocal of these integers. Then reduce these to the smallest set of integers h, k, and l.
  - (3) Label the plane as [hkl].

Example)

- The plane on the right figure has intercepts at 2a, 4b, and 1c.
- The reciprocals are ½, ¼, and 1.
- These are reduced to 2, 1, and 4.
- Therefore the plane has the label of [214].



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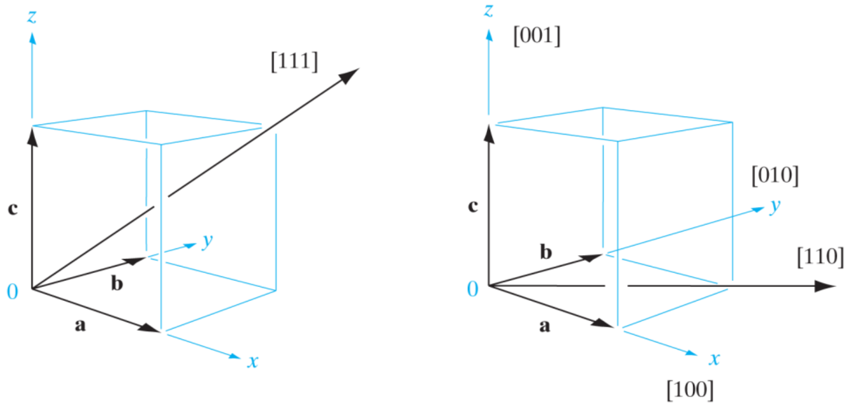
Band Structure in Different Directions



Left Figure. Crystal directions in the cubic lattice

- Crystal directions have the same relationship with the labeling of the plane. In other words, [214] plane has the crystal direction of [214].
- The body diagonal of cubic lattice (above, left frame) has [111] direction.
- Many directions of the lattice are equivalent. The crystal axes in the cubic lattice [100], [010], and [001] are all equivalent and are called <100> directions. (See above figure, on the right frame)
- [100], [110], [111] are different.

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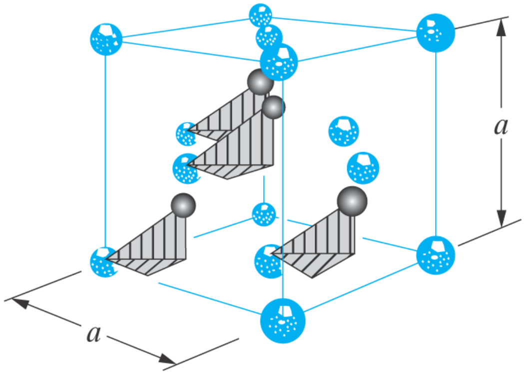
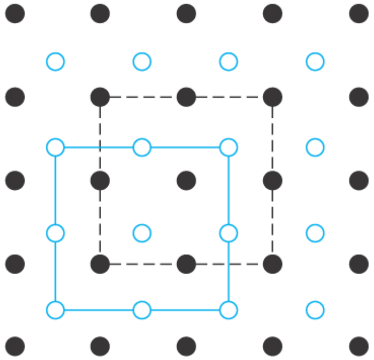
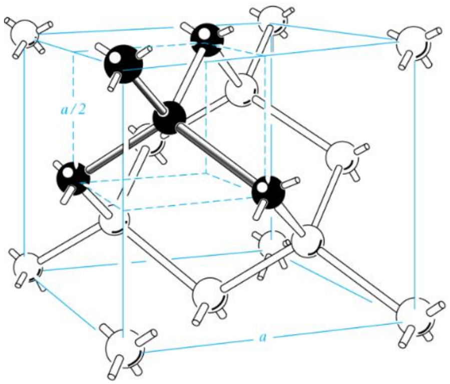
Silicon: Diamond Lattice







- Many important semiconductor crystals (Si, Ge, C) have diamond lattice structure, which is composed of two fcc lattices.
- The diamond structure can be thought of as an fcc lattice with an extra atom placed at a/4+b/4+c/4 from each of the fcc atoms.
- Above figures show diamond lattice structure: a unit cell of two fcc structures (left), its top view (center) and 3D view (right).

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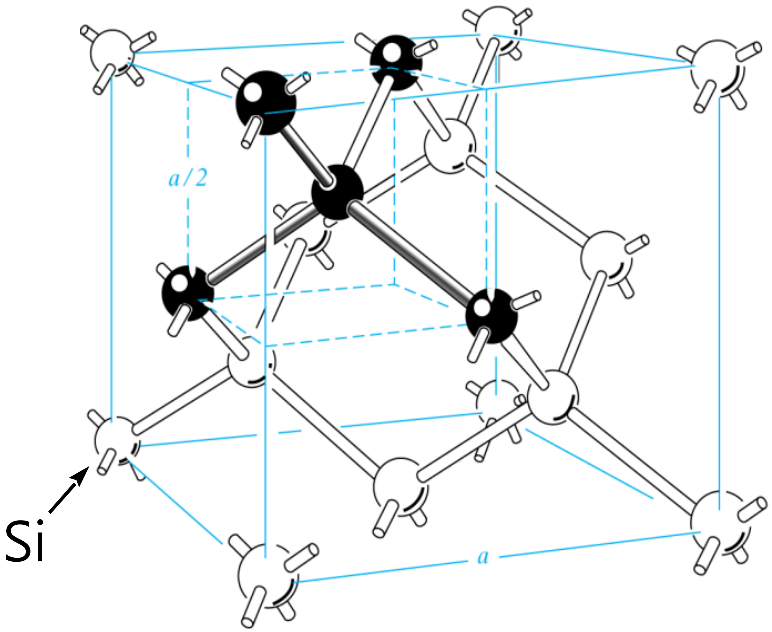
Compound: Zinc Blend Lattice



- Many important III-V compound semiconductor crystals (GaAs, GaN, InP) have zinc blend lattice structure, which is similar with diamond structure.
- The basic structure (two misaligned fcc structures) is same. But if the atoms of two fcc structures are same, then it is diamond structure, while if two are different, then it is zinc blend structure.
- Compound semiconductors are important for optoelectronic devices, such as light emitting diodes or photodetectors, and high speed devices (MESFET).

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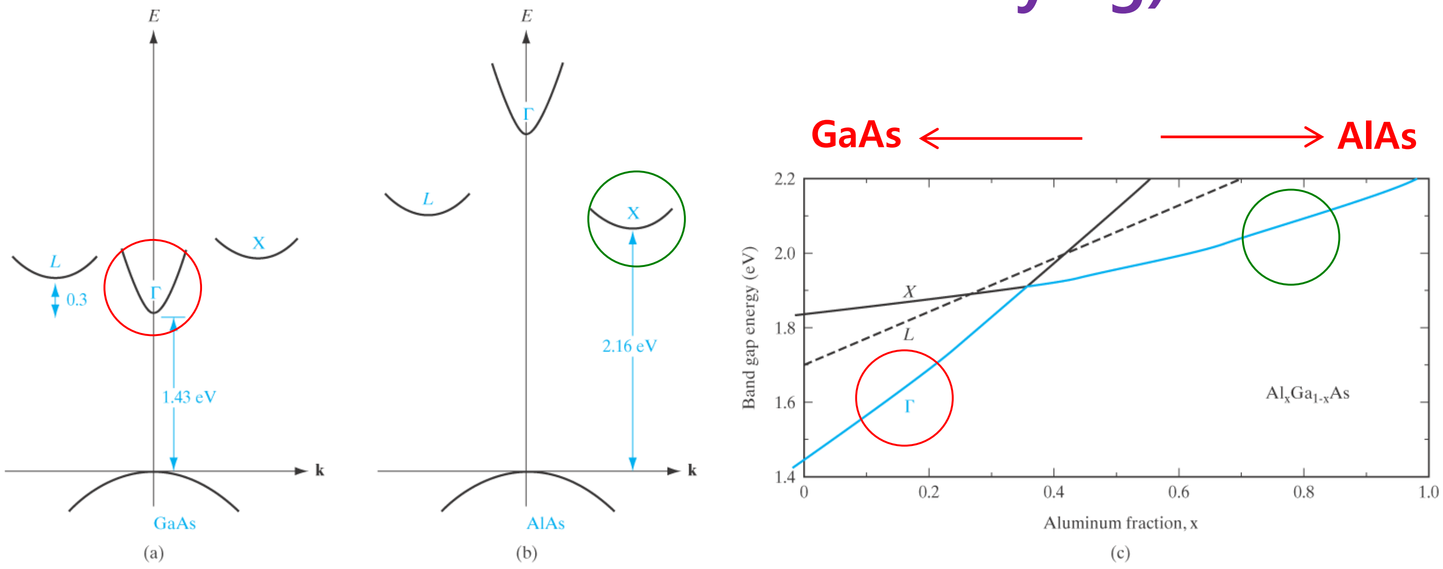
Direct and Indirect

- E-k diagram: Allowed values of E vs k (wave vector, momentum of e^- and h^+) can be plotted.
- Since the **periodicity of most crystal lattices is different in various directions** of electron movement, relationship between E and k can be plotted as above.
- **Direct gap material** (like GaAs) has the conduction band minimum and valence band maximum at the same k, while indirect gap material (like Si) has them at different k.
- In the case of **indirect gap**, the electron should change the direction of movement to move between minimum and maximum and thereby involves with momentum change in k.
- In direct gap, an electron in CB falls to an empty space of VB and gives off photons (light).
- In indirect gap, the momentum changes are needed and phonon (lattice vibration) involves, which emits energy change as a heat instead of light.
- Generally, optoelectronic devices, like LED, are made of direct gap materials.

Band Change in Alloy

- Different compound semiconductors have different band structures, which can be tuned by alloying them.
- GaAs and AlAs can be alloyed to make $Al_xGa_{1-x}As$.
- Depending on the Al fraction in alloy the band gap structure changes from indirect gap (AlAs) to direct gap (GaAs), as shown in the following diagrams.

- **Overall, smaller (larger) lattice results in larger (smaller) bandgap E**
- **GaAs and AlAs do not have much lattice mismatch (less defects in alloying)**



(a) (b) (c)

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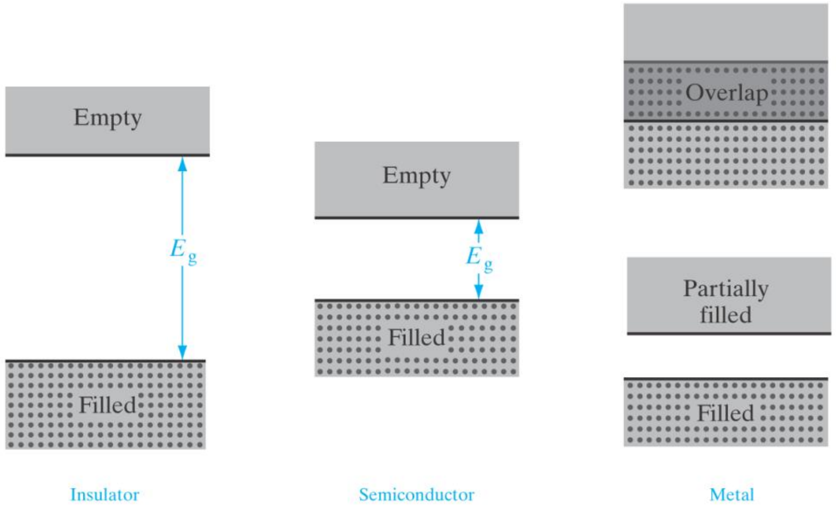
Carriers: Electrons and Holes



- Semiconductors differ from metals and insulators by the fact that they contain an **"almost-empty" conduction band and an "almost-full" valence band** (> 0 K). This also means that we will have to deal with the **transport of carriers in both bands**.
- To facilitate the discussion of the transport in the almost-full valence band of a semiconductor, we will introduce the concept of **holes**.
- The concepts of holes is introduced in semiconductors since **it is easier to keep track of the missing electrons in an "almost-full" band**, rather than keeping track of the actual electrons in that band.
- Holes are missing electrons. They behave as particles with the same properties as the electrons would have when occupying the same states except that they carry a positive charge. This definition is illustrated further with next slide, which presents the energy band diagram in the presence of an electric field.

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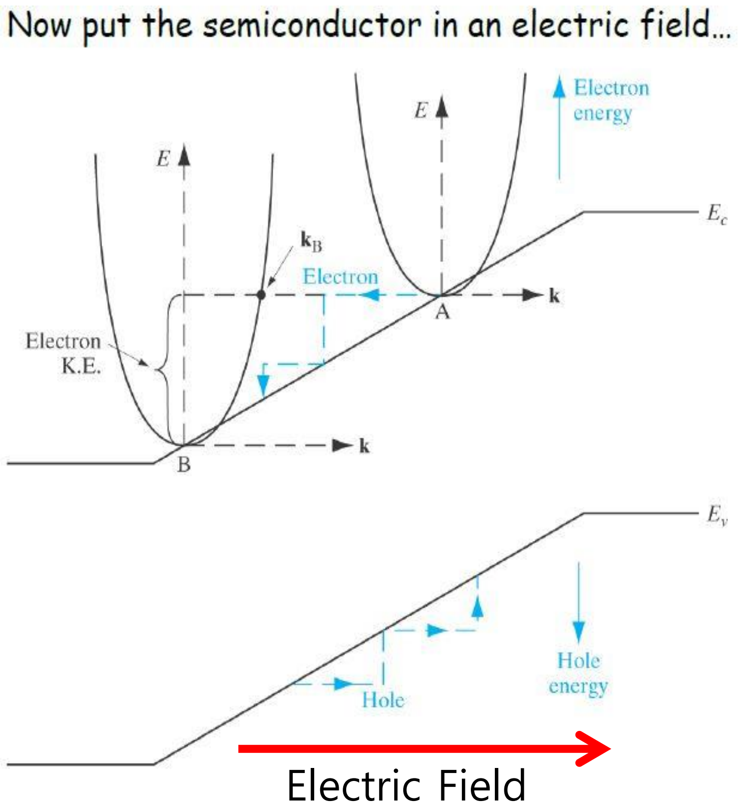
Motion of Carriers: Electric Field



- (E, k) diagram is a **plot of the total electron energy (potential + kinetic) as a function of the crystal-direction dependent electron wave vector** (k, which is proportional to the momentum).
- Different crystal direction has different E-k diagram
- Therefore the **bottom of the conduction band (where k=0) corresponds to zero electron velocity or kinetic energy and simply gives the potential energy at that point**. (left)
- Energies higher in the band than the minimum k point corresponds to **additional kinetic energy** of the electron (potential+kinetic E).
- **Since the band edge corresponds to the electron potential energy, the variation of the band edge in space is related to the electric field** at different points of semiconductor.
- In the left diagram, electron at location A sees an electric field given by the slope of the band edge (potential energy), and gains kinetic energy (at the expense of potential E) by moving to point B (less potential E, more kinetic E).
- **The slope of band edge represents local electric field** of each point.

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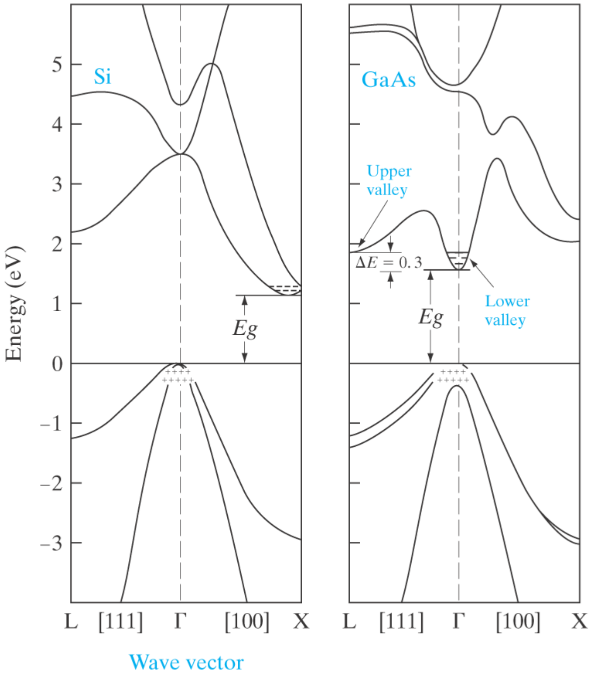
Mobility: Effective Mass



Group	Material	m_n^*	m_p^*
IV	Si (4K)	1.06	0.59
	Si (300K)	1.09	1.15
	Ge	0.55	0.37
III-V	GaAs	0.067	0.45
	InSb	0.013	0.6
II-VI	ZnO	0.29	1.21
	ZnSe	0.17	1.44

- The **electrons** in a crystal are not completely free, but instead <u>**interact with the periodic potential of the lattice**</u>. The <u>interacting force is different in different materials and different directions in one material</u>.
- A particle's effective mass (often denoted m*) is the <u>**mass that it seems to have when responding to forces**</u>. (higher interaction ~ heavier effective mass)
- For electrons or holes in a solid, effective mass is usually stated in units of the true mass of the electron m_e, 9.11×10^{-31} kg.

$$m^* = \frac{(h/2\pi)^2}{d^2E/dk^2}$$

$$\boxed{\mu_n = \frac{q\tau_c}{2m_n^*}}$$

scattering

high curvature at CB minimum and VB maximum in E-k diagram ~ low effective mass

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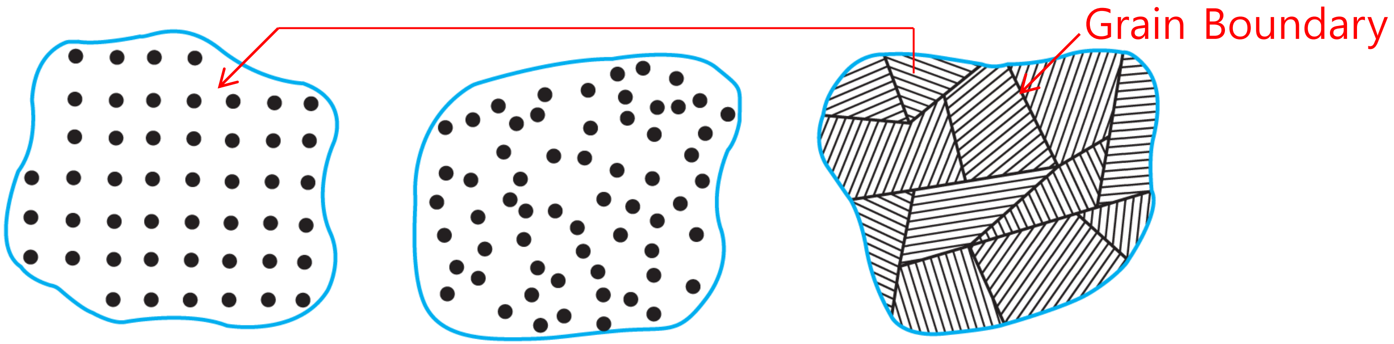
Crystal Structures



(a) Crystalline (b) Amorphous (c) Polycrystalline

Microprocessor, DRAM Thin film PV, LCD Si bulk PV, OLED

Grain boundaries

- interfaces where crystals of different orientations meet
- crystals on each side of the boundary being identical except in orientation
- grain boundary areas contain defects, dislocations, and impurities
- Since grain boundaries are defects in the crystal structure, they tend to decrease the electrical and thermal conductivity of the material.
- Grain boundaries are in general only a few nanometers wide. In common materials, crystallites are large enough that grain boundaries account for a small fraction of the material.
- In the limit of small crystallites, the material ceases to have any crystalline character, and thus becomes an amorphous solid.

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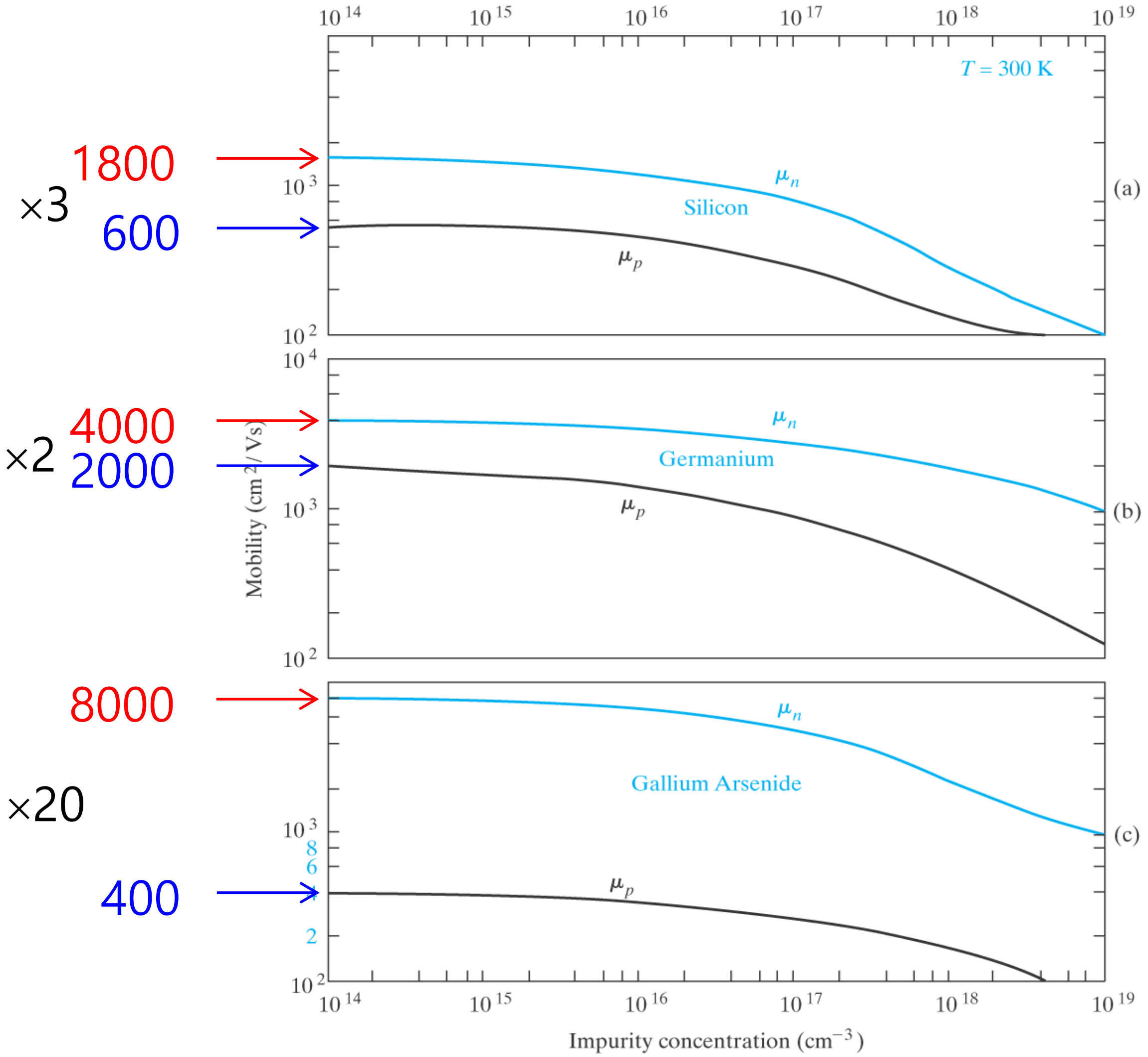

Figure 3.23

Variation of mobility with total doping impurity concentration ($N_a + N_d$) for Ge, Si, and GaAs at 300 K.

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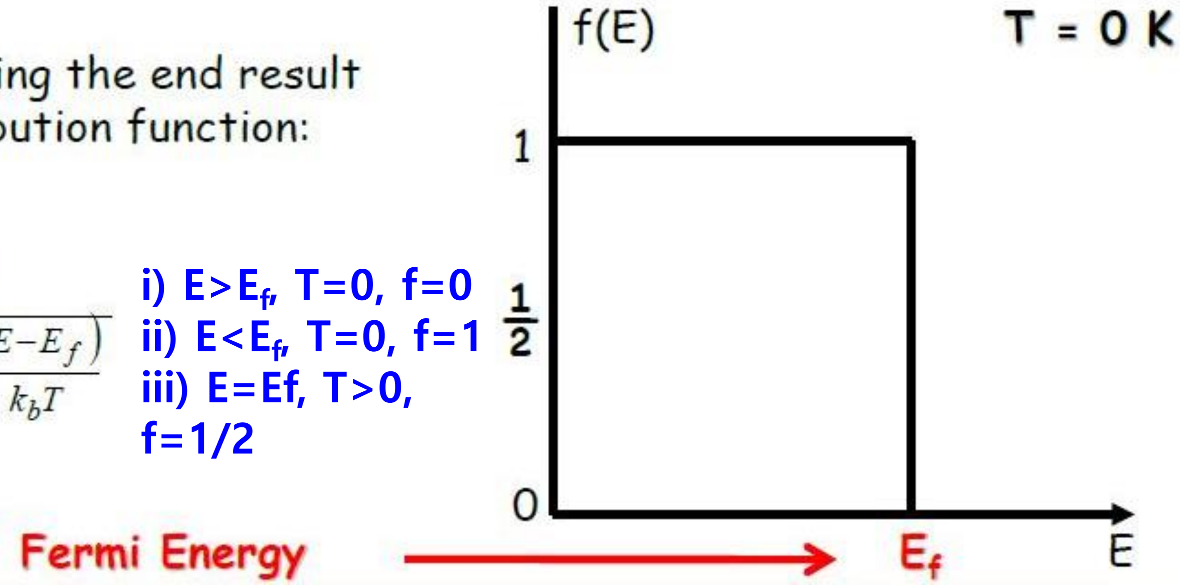
Fermi Level

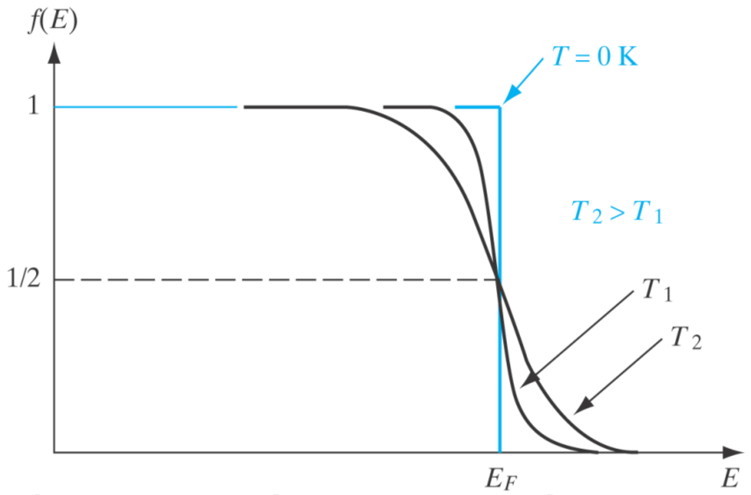
Mathematically speaking the end result is a probability distribution function:

$$f(E) = \frac{1}{1 + e^{\frac{(E - E_f)}{k_b T}}}$$

i) $E > E_f$, $T = 0$, $f = 0$
ii) $E < E_f$, $T = 0$, $f = 1$
iii) $E = Ef$, $T > 0$, $f = 1/2$



- At temperatures higher than 0K, some probability exists for states above the Fermi level to be filled.
- In applying Fermi-Dirac distribution, f(E) is the probability of occupancy of an available state at E.
- In intrinsic materials, $f(E_F) = ½$, since the number of electrons and holes are same.
- E_F is the energy level where $f(E_F) = ½$.



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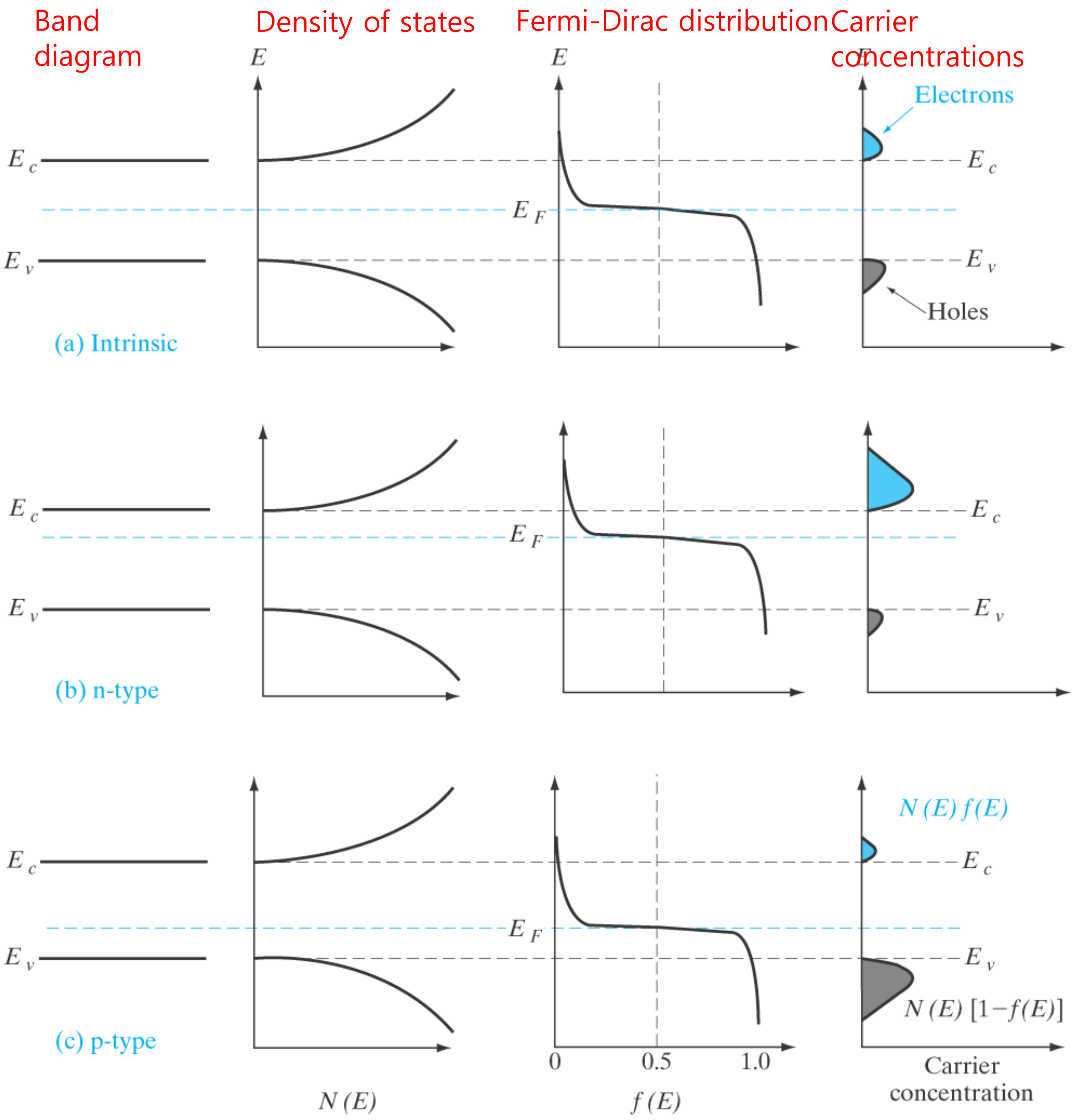
- Compare three cases (intrinsic, n and p type) in one charts
- Band diagram, Density of states, Fermi-dirac distribution and carrier concentrations for intrinsic, n type and p type materials



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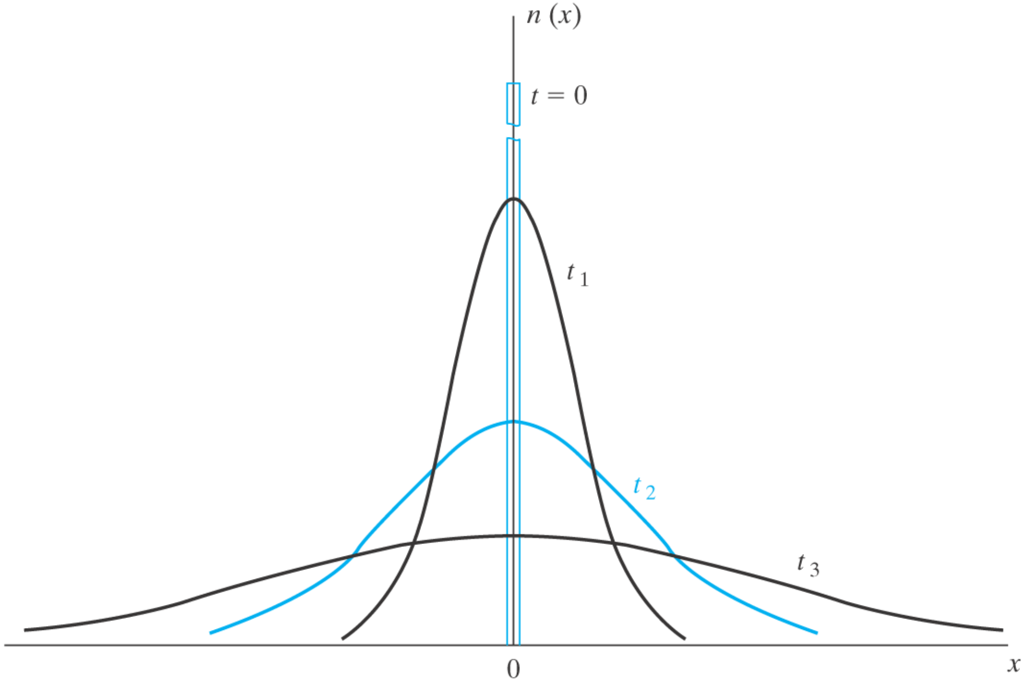
Diffusion of Carriers

- **Carriers in a semiconductor diffuse in a carrier gradient by random thermal motion and scattering from the lattice and impurities, from high concentration to low concentration.**

  Cf) Drift: driving force – electric field

  Diffusion: driving force – concentration difference

- **Example: A pulse of excess electrons injected at x=0 at time t=0 will spread out in time as shown in Fig. 4.12.**



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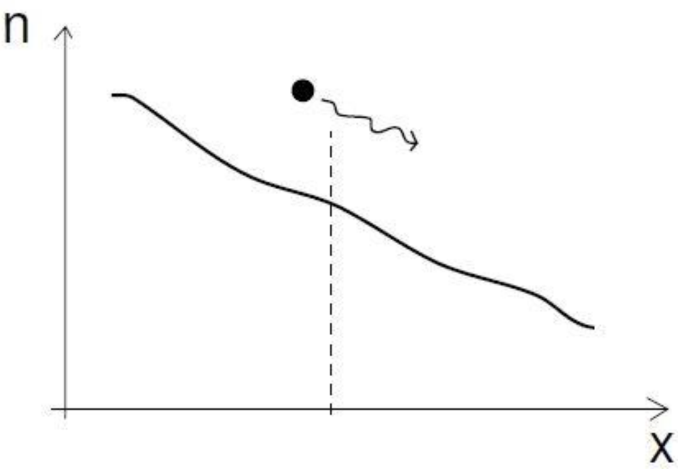
Diffusion = particle movement (flux) in response to concentration gradient



Diffusion flux ∝ - concentration gradient

Flux ≡ number of particles crossing a unit area per unit time [$\mathrm{cm^{-2} \cdot s^{-1}}$]

For Electrons:

$$F_n = -D_n \frac{dn}{dx}$$

For Holes:

$$F_p = -D_p \frac{dp}{dx}$$

Diffusion current density = charge × carrier flux

$$J_n^{diff} = qD_n \frac{dn}{dx}$$

$$J_p^{diff} = -qD_p \frac{dp}{dx}$$

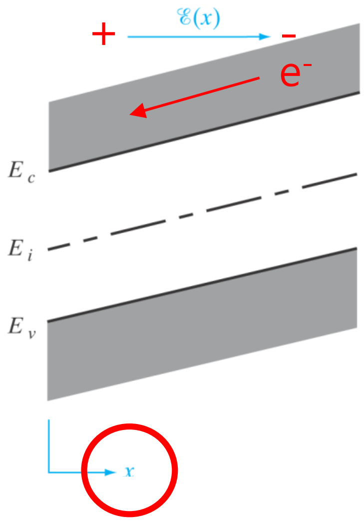
- If an electric field is present in addition to the carrier gradient, the current densities will have a drift component and a diffusion component.
- Therefore the total current density is as follows:

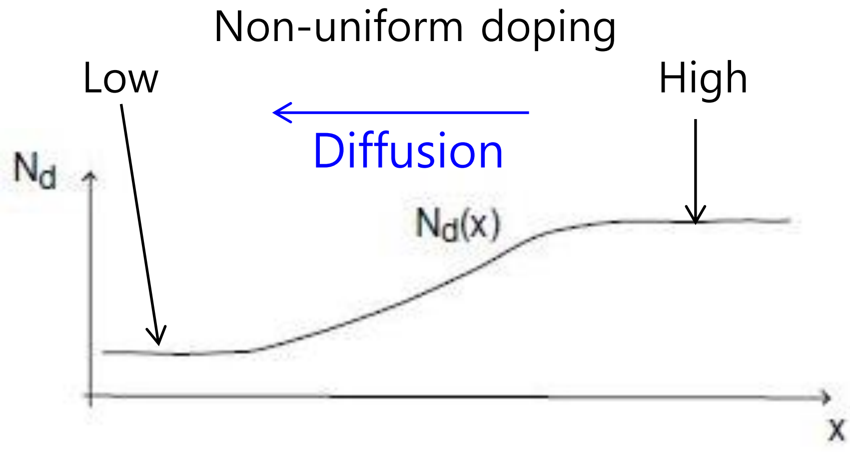
$$\boxed{\begin{aligned} J_n &= J_n^{drift} + J_n^{diff} = qn\mu_n E + qD_n \frac{dn}{dx} \\ J_p &= J_p^{drift} + J_p^{diff} = qp\mu_p E - qD_p \frac{dp}{dx} \\ J_{total} &= J_n + J_p \end{aligned}}$$

- Majority carriers mainly contribute through drift, while minority carriers contribute through diffusion.
- **The concentration of majority current can be much larger than minority current, but the concentration gradient of minority current can be significant.**
- **Therefore diffusion current by minority carriers sometimes is comparable to drift current by majority carriers (ex. Diffusion – diode, Drift – transistor)**

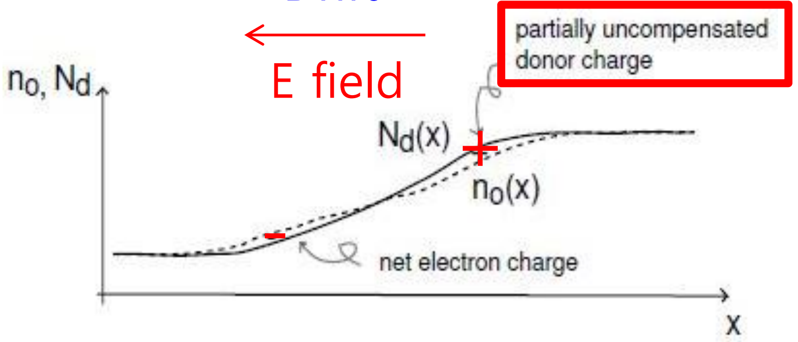
- It is important to discuss the influence of electric field on the energies of electrons in the band diagrams.
- Let's assume E field E(x) in the x direction, then the energy band bending will be as shown in the right figure (Fig. 4.15).
- From the definition of electric field, E(x) is as follow:

$$E(x) = -dV/dx \text{ or } -\Delta V/l$$





Drift



- For non-uniform doping in equilibrium (no net current), the carrier concentration gradient (due to non-uniform doping) make a diffusion current, while a built-in electric field (by uncompensated charges) makes a drift current.
- For both electron and hole components, the net current is zero and thus drift and diffusion current are canceled out.

$$J_n(x) = J_n^{\text{drift}}(x) + J_n^{\text{diff}}(x) = 0$$

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Summary

We have learned fundamental concepts (blue headings below) for electronic device (diodes, transistors, circuits) study.

(1) bonding, anti-bonding
(2) band structure (conduction, valence band, band gap)
(3) direct gap and indirect gap materials
(4) electron, hole and their pairs
(5) bands in electric field
(6) intrinsic and extrinsic materials

Fundamental Concepts

(7) p type and n type doping
(8) Fermi level
(9) temperature effect on semiconductor
(10) carrier drift
(11) mobility, resistivity and scattering
(12) carrier diffusion

More Applied Concepts

The questions, when we begins these chapters, were…

(1) How to make different charge distribution: n and p type regions
(2) How to make carriers(charges) move(transport) from one location to the other in a controlled way (by applying bias or by making carrier concentration gradient)