Session 2: Solids - Crystals

Solid State Devices:

History

Metal semiconductor contact (1874) → Light emitting diode (1907) → Crystal rectifier (1906-16) → Quantum theory (1925) → Quantum theory of Solids (1930-1940) → Bi-Polar Transistor (1947)

→ P-n Junction (1949) → Thyristor (1952) → Solar Cell (1954) → Heterojunction polar transistor (1957) → Tunnel diode (1958) → Hybrid integrated circuit (1959)

→ Monolithic integrated circuit (1959) → MOSFET (1960) → Laser (1962) → Heterostructure laser (1963) → Transferred-electron diode (TED) (1963) → CMOS (1963)

→ IMPATT diode (1965) → MESFET (1966) → DRAM (1967) → Non-volatile semi-conductor memory (1967) → CCD (1970) → 4004 Micro-Processor (1971)

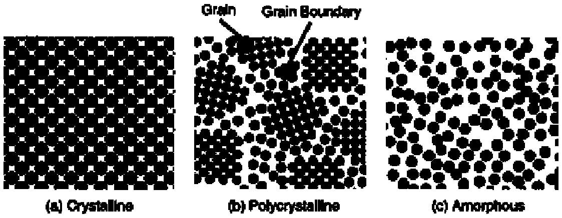
→ Resonant tunneling diode (1974) → LEDs (1975) → MODFET (1980) → Room temperatur single-electron memory cell (1994) → Blue LEDs (2000) → 20 nm MOSFET (2001)

SSI (1958-64) → MSI (1964-68) → LSI (1968-75) → VLSI (1975-90) → VHSIC (1980-1990) → Bio-Chips (???)

States of the matter

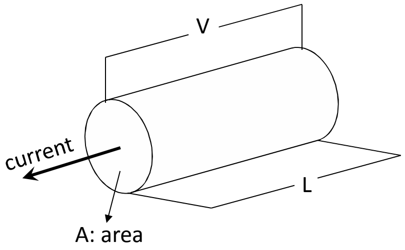
? Why Solid State?

1. Solid: density ~ 10^{22} /cm^3
   - 1. a: Crystal: long range order (lattice + basis) {Ex: Epitaxial silicon and diamond}
   - 1. b: Polycrystal: short range order (µm ~ 10µm) {Ex: Most metals (Al, Cu) Ploy-Si}
   - 1. c: Amorphous: no order {Example: Glasses like SiO2}



2. Liquids: no order, takes the shape of the container, weak bounds; density ~ 10^{19} /cm^3
3. Gases: no order, no bounds between molecules
4. Liquid crystals: atoms mobile, type of long range order Applications: LCDs
5. Plasma: Ionized gas/liquid {Ex: Sun, Aurora, Lightning, (RIE, Sputtering, PECVD)}

Resistivity



Ohm's law

$$R = \frac{V}{I} \rightarrow \rho = R\frac{A}{L}$$ resistivity

Resistivity is characteristic of the material

Art of VLSI design is:
to put together materials with different resistivity's next to each other to perform a certain task.

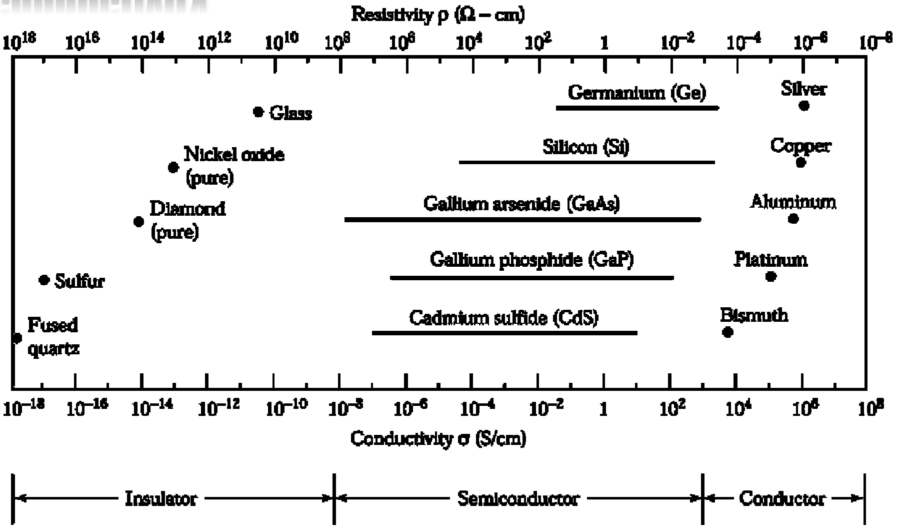
Conductor

$$Al, Cu \longleftrightarrow SiO_2$$

$$\rho_{Al} \approx 10^{-6}\ [\Omega cm] \qquad \rho_{SiO_2} \approx 10^{16}\ [\Omega cm]$$

Insulator

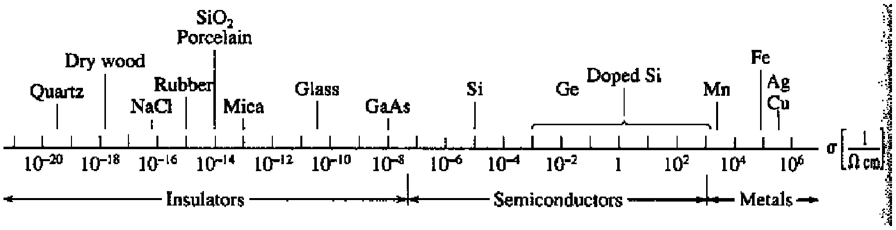
conductivity



Typical range of conductivities for insulators, semiconductors, and conductors.

Semiconductors

Insulators 10^5 [Ωcm] **Semiconductors** 10^{-2} [Ωcm] **Conductors**

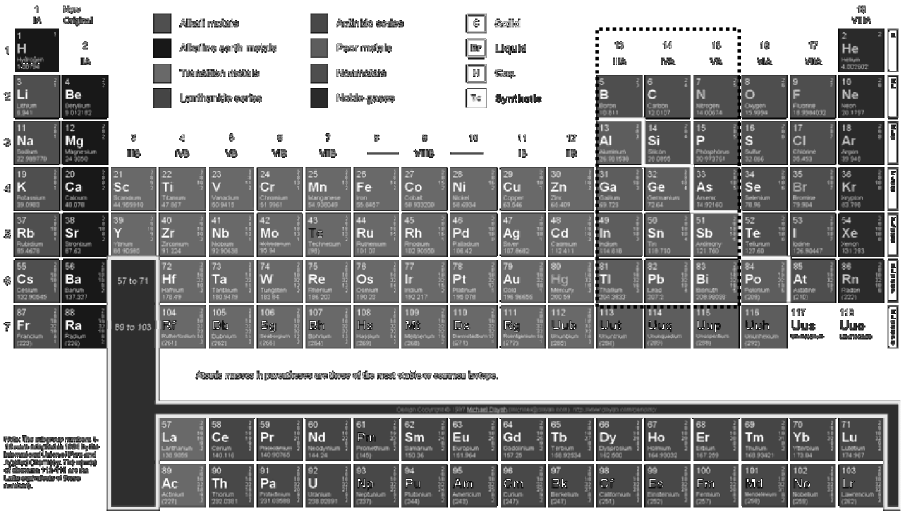


? Is the “resistivity” the only difference between semiconductors and conductor / insulators ?

In semiconductors: conductivity is controllable

In conductors: carriers are “electrons”
In semiconductors: carriers are “electrons” + “holes”

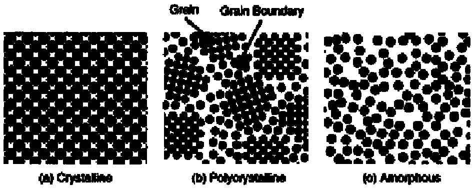
Periodic Table of the Elements



Abbreviated periodic table

1 IA 1A							18 VIIIA 8A
1 **H** 1.008	2 IIA 2A	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 **He** 4.003
3 **Li** 6.941	4 **Be** 9.012	5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31	13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
9 **K** 39.10	30 **Zn** 65.39	31 **Ga** 69.72	32 **Ge** 72.59	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.80
37 **Rb** 85.47	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
55 **Cs** 132.9	80 **Hg** 200.5	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** (210)	85 **At** (210)	86 **Rn** (222)

Solids



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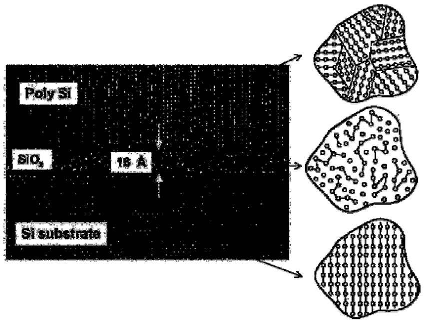
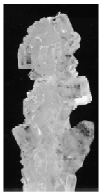


A Little History - Crystal Structure

Solids tend to form ordered crystals

Rock Salt

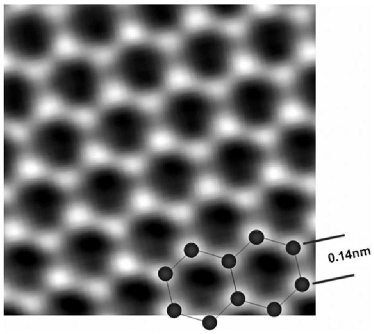
Rock Candy



Mineralogists have been familiar with crystal structures since 18th century.
1912: Diffraction of x-rays by a periodic array.
Today : Condensed matter physics long way to go …..

Properties (mechanical, electrical, optical and thermal properties all affected) of solids depends on their structure

Crystal Lattices



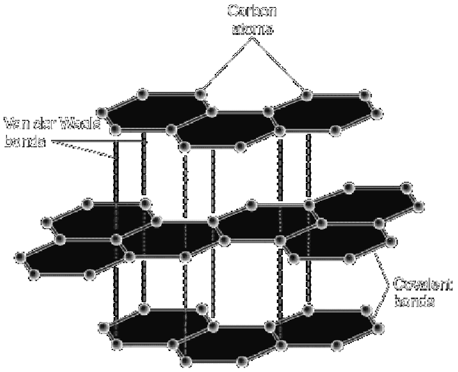
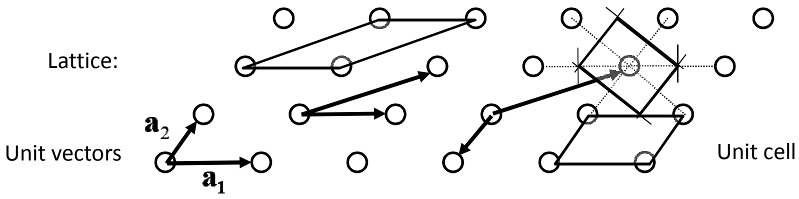


Image of graphene in a
transmission electron microscope.

Crystal Structures

Ideal Crystal: Infinite repetition of identical structural units in space.

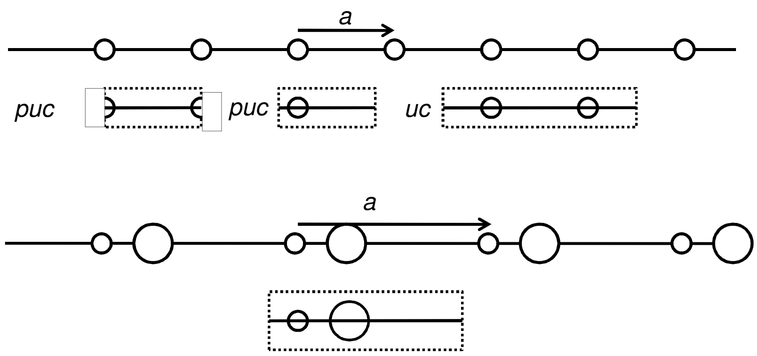


$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$$

Bravais lattice: is the set of points defined by $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ as n_i is integer.
Shortest possible $\mathbf{a}_i$ gives us primitive vectors.
The volume cell enclosed by the primitive vectors is called the primitive unit cell.

Crystal structure = Lattice + Basis

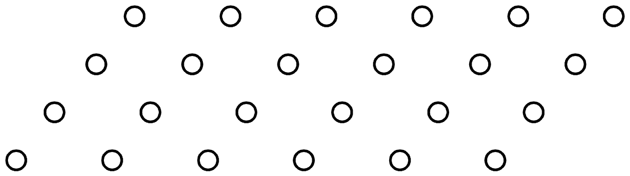
One-Dimensional Lattices



Crystal Structures

Ideal Crystal: Infinite repetition of identical structural units in space.

Lattice:



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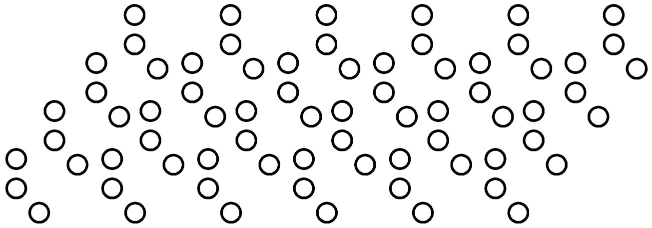
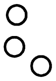
Lattice, Basis

Ideal Crystal: Infinite repetition of identical structural units in space.

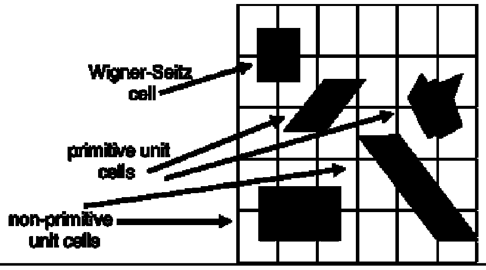


Crystal structure = Lattice + Basis

Basis

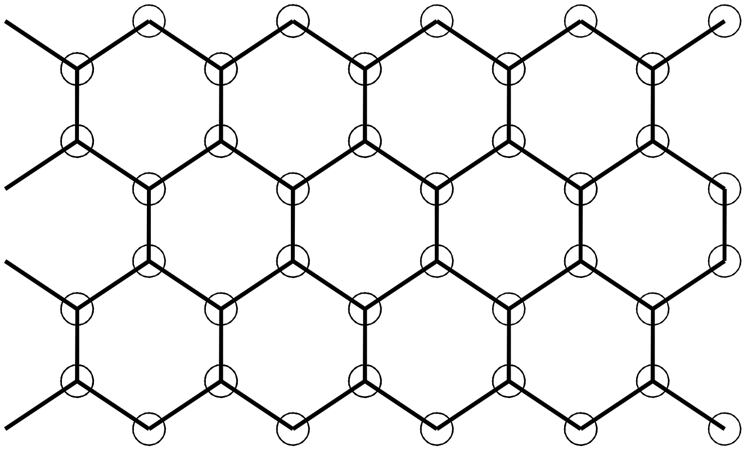


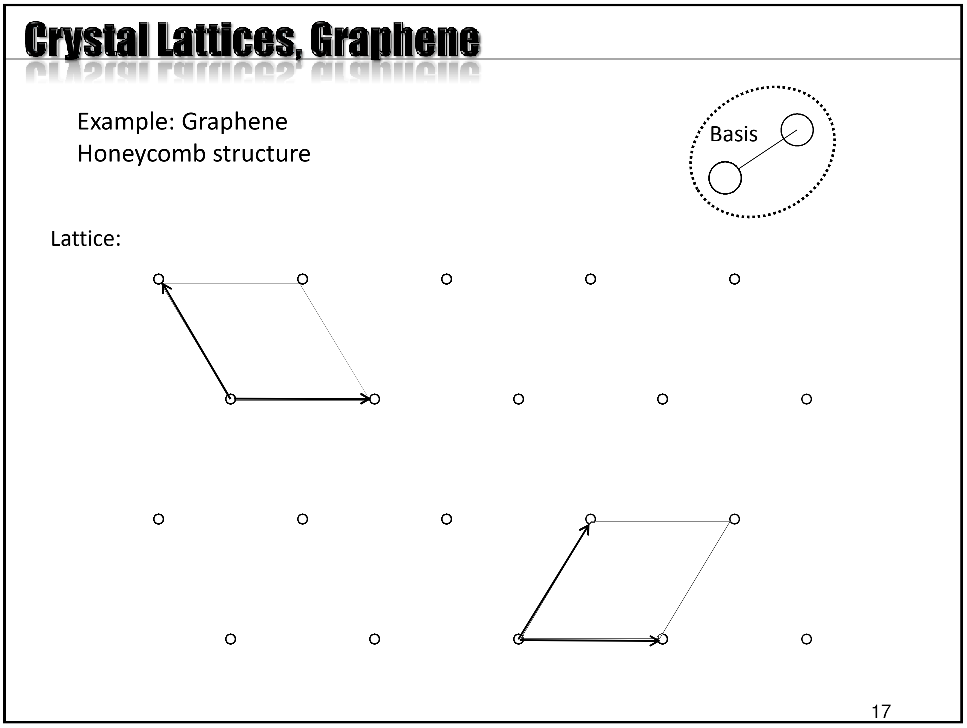
The basis consists of the simplest arrangement of atoms which is repeated at every point in the lattice to build up the crystal structure



Crystal Lattices, Graphene

Example: Graphene
Honeycomb structure

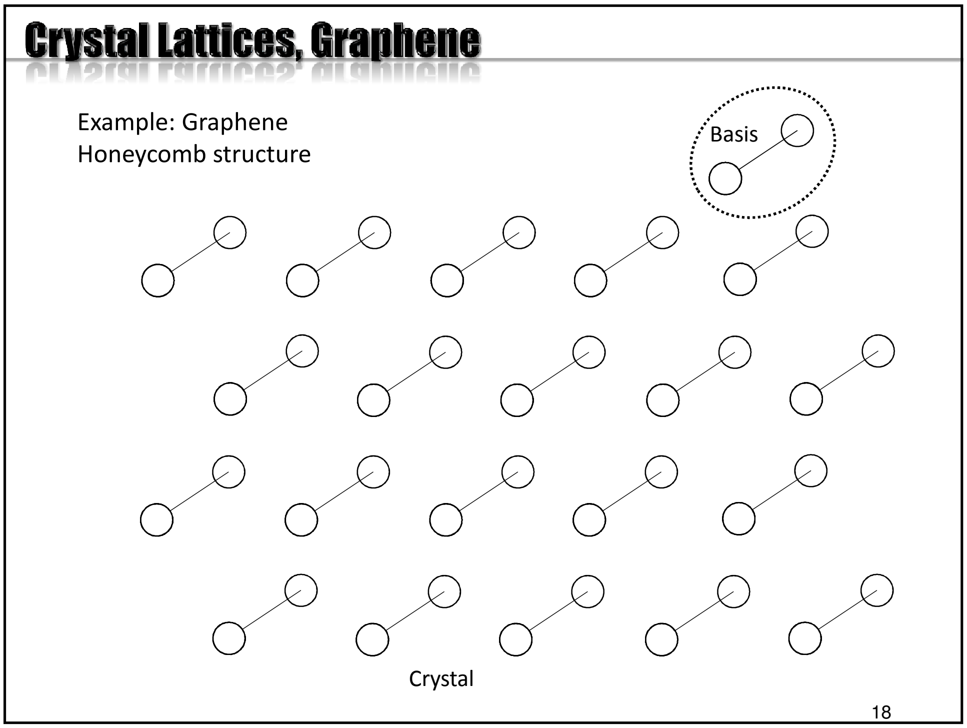




Crystal Lattices, Graphene

Example: Graphene
Honeycomb structure

Lattice:



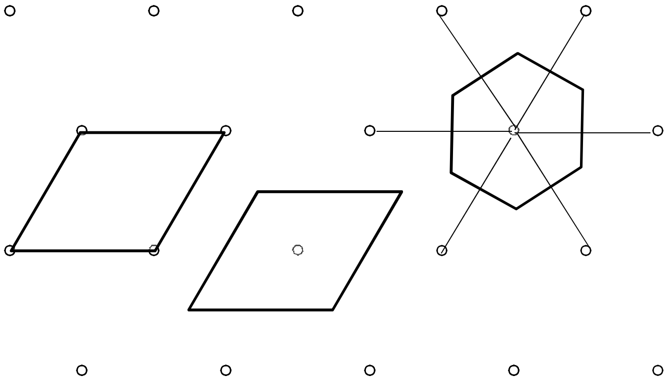
Crystal Lattices, Graphene

Example: Graphene
Honeycomb structure

Crystal

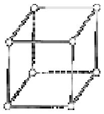
Crystal Lattices, Graphene

Example: Graphene
Honeycomb structure

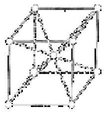


Cubic Lattices

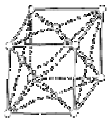
Simple cubic (SC)



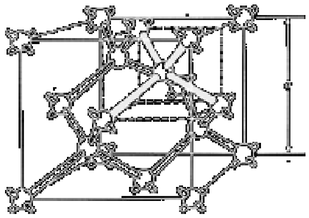
Body-centered cubic (BCC)



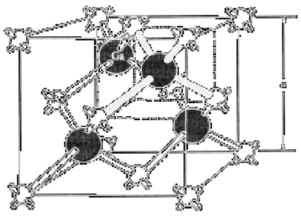
Face centered cubic (FCC)



Diamond Lattice



Zinc Blend Structure



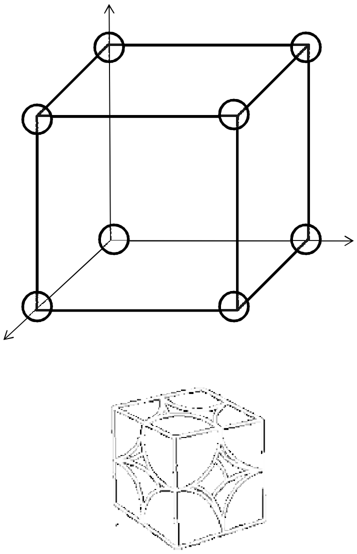
Simple Cubic

Example:
alpha polonium

Coordination Number (# of nearest nbs.) =

# of atoms/cell =

Packing fraction =



Body Centered Cubic

Example:

Sodium,

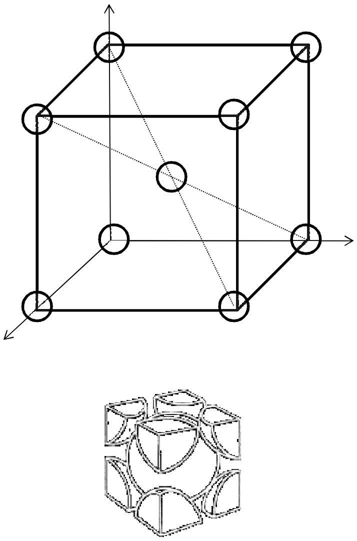
Molybdenum,

Tungsten

Coordination Number (# of nearest nbs.) =

# of atoms/cell =

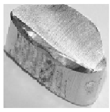
Packing fraction =

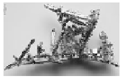


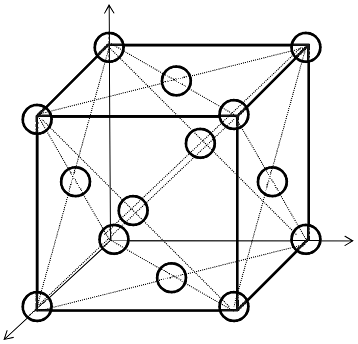
Face Centered Cubic

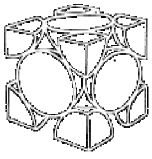
Example:

Aluminum, Copper, Gold, Silver,









Coordination Number (# of nearest nbs.) =

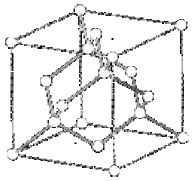
# of atoms/cell =

Packing fraction =

Diamond Lattice

Example:

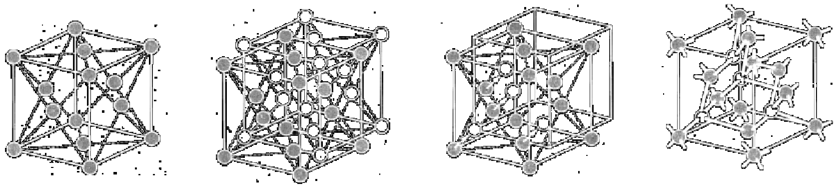
Silicon, Germanium, Carbon



Coordination Number (# of nearest nbs.) =

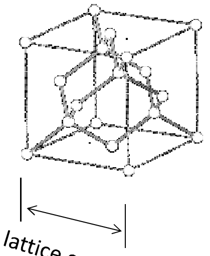
# of atoms/cell =

Packing fraction =



Diamond Lattice

Example:
Silicon, Germanium, Carbon



Coordination Number (# of nearest nbs.) =

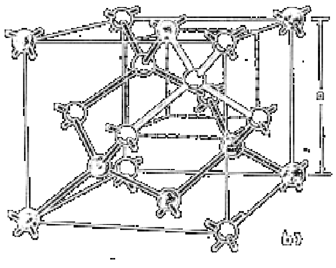
# of atoms/cell = 8

Packing fraction =

Cell volume:
$(.543\ \text{nm})^3 = 1.6 \times 10^{-22}\ \text{cm}^3$

Density of silicon atoms
= (8 atoms) / (cell volume) = 5×10^{22} atoms/cm^3

Zinc Blend Structure



III-V semiconductors, important for optoelectronics.

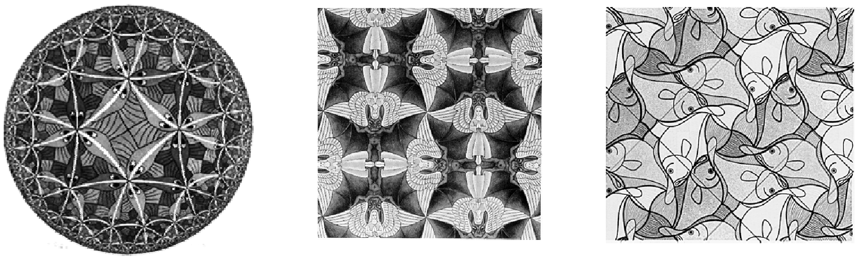
GaAs, InP,
InGaAs,
InGaAsP,……..

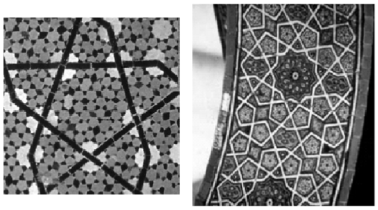
For GaAs:

Each Ga surrounded
By 4 As, Each As
Surrounded by 4 Ga

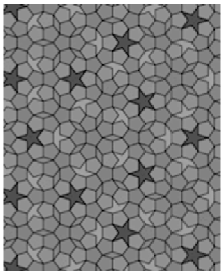
Non-Bravais Lattices

MC Escher





Islamic art



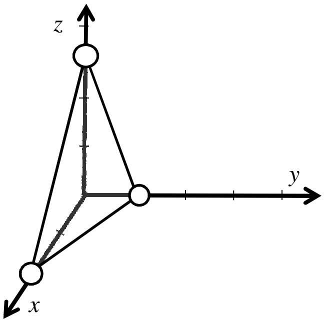
Penrose Tilings

“Quasi-periodic”
(Lower-D Projections
of Higher-D periodic
systems)

Miller Indices

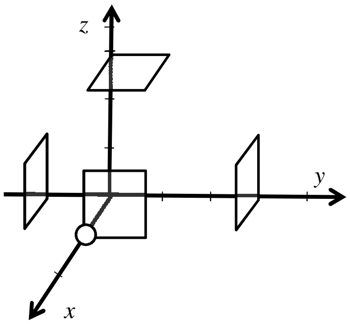
A method to label distinct planes and direction within a crystal structure.
steps:

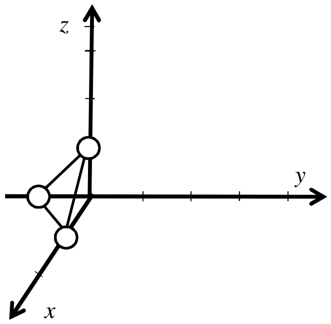
1. Note where the plane to be indexed intercepts the axes (chosen along unit cell directions). Record result as whole numbers of unit cells in the x, y, and z directions, e.g., 2, 1, 3.
2. Take the reciprocals of these numbers, e.g., 1/2, 1, 1/3
3. Convert to whole numbers with lowest possible values by multiplying by an appropriate integer, e.g., x6 gives 3, 6, 2.
4. Enclose number in parentheses to indicate it is a crystal plane categorization, e.g., (3,6,2)



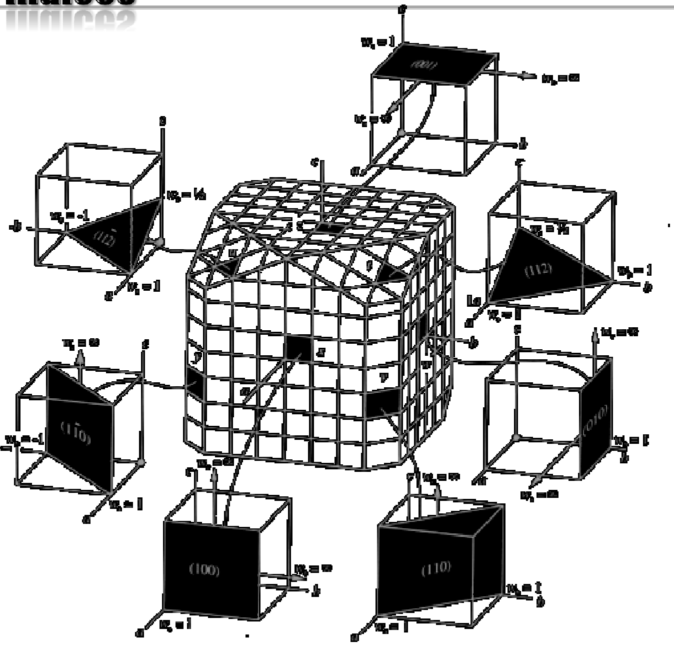
Miller Indices

Planes parallel to a unit cell coordinate axis are viewed as intercepting the axis at infinity, so have an associated Miller index in that direction of zero, e.g., (100) plane. Planes intersecting along the negative axis use a bar over the index rather than a negative sign, e.g., $\bar{1}$ rather than -1, e.g., $(1\bar{1}1)$.
Groups of equivalent planes,($(100), (010), (001), (\bar{1}00), (0\bar{1}0), \text{ and } (00\bar{1})$ all equivalent because rotation about the 3 fold axes on the cube diagonals maps the various faces into one another, making the planes equivalent) are notated in curly brackets, i.e., {100} for the above set of equivalent planes.





Miller Indices



Miller Indices

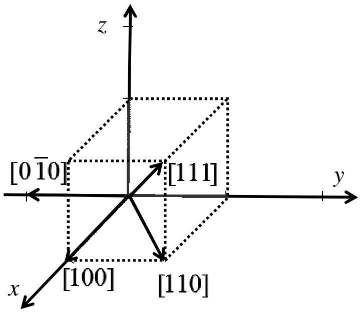
Similar procedure can be used to define Miller indices for directions.

1. Set up a vector of arbitrary length in the direction of interest (must be a crystal direction, i.e., connecting two crystal points)
2. Decompose the vector into its basis vector components in the a, b, and c directions
3. Convert the resulting numbers to the lowest possible set of integers by multiplying by an appropriate number

Directions are notated using square brackets, e.g., $[1\bar{1}1]$

For cubic crystals, directions perpendicular to particular crystal planes can be indexed using the same index as the plane. Sets of equivalent directions are specified by triangular brackets, e.g., $\langle 100 \rangle$

[h,k,l] ⊥ (h,k,l)

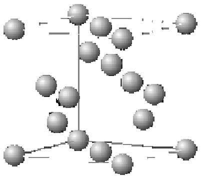


Miller Convention Summary

Convention	Interpretation
(hkl)	Crystal plane
{hkl}	Equivalent planes
[hkl]	Crystal direction
⟨hkl⟩	Equivalent directions

Crystallographic Planes

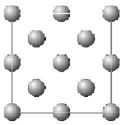
Unit cell



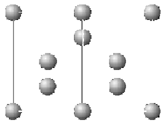
a=5.431 °A

5×10^{22} atoms/cm^3

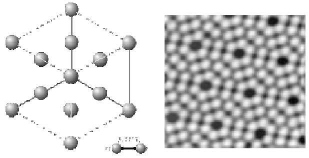
<100> view



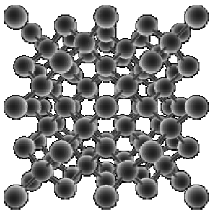
<110> view



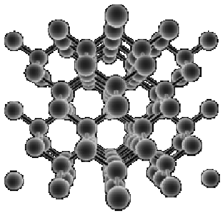
<111> view

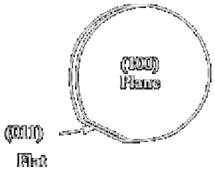


(100)



(110)





Silicon wafers are usually cut along the (100) plane with a flat or notch to help orient the wafer during IC fabrication.

K-space

The reciprocal lattice of a lattice (usually a Bravais lattice) is the lattice in which the Fourier transform of the spatial function of the original lattice (or direct lattice) is represented. This space is also known as momentum space or less commonly k-space

real space primitive vectors:	$(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$	sc	fcc	bcc
reciprocal lattice primitive vectors:	$(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$	sc	bcc	fcc

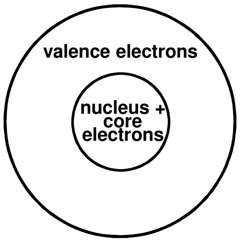
$$V = \mathbf{a}_1 \bullet (\mathbf{a}_2 \times \mathbf{a}_3) \qquad \mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V} \qquad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V} \qquad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

All features are periodic with periodicity of the lattice, just like Fourier transform it can be written as

$$\varphi(\mathbf{r}) = \varphi(\mathbf{r} + \mathbf{a}_\mathbf{n}) = \sum \varphi_b e^{i\mathbf{b}\times\mathbf{r}} \quad \text{where} \quad \mathbf{a}_\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Atomic bonding

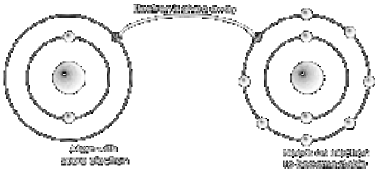
Atoms vibrate with small amplitudes about fixed equilibrium positions. We assume that atoms are fixed, unless phonons are considered.
Atoms look like outer valence electrons orbiting around the core. Core consists of nucleus plus inner core electrons



Ionic bond: Na^+Cl^-
Covalent bond: sharing e^- to complete an octet
H need only one atom to complete the octet and therefore we only have H_2.
Silicon needs 4 e^- and so can bond to four other Si atoms, forming a crystal.
Metallic bond:
Van der Waals:

Ionic bonding

Complete transfer of electrons from one atom (usually a metal) to another (non metal ion) (compounds only, not elemental solids). Bond comes from electrostatic attraction between ions.

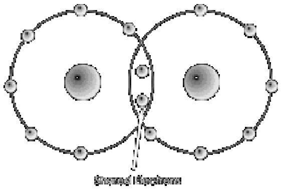


$$Na + Cl \rightarrow Na^+ + Cl^- \rightarrow NaCl$$

All ionic compounds have a degree of covalent bonding. The larger the difference in electronegativity between two atoms, the more ionic the bond is.
- Bond is strong (high melting point, large elastic modulus)
- Not directional (high density, high coordination number)
- Compounds only
- Good insulators (except near melting point)
- Transparent up to UV (strong bonds → electrons need a lot of energy to become free)

Mathematical form: Energy ~ 1/r, Example: Sodium Chloride

Covalent Bonding

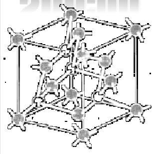


Equal sharing of electrons between atoms → both atoms have full shells (Example: Diamond, Silicon)

Note continuum of behavior, ionic → covalent (e.g. III-V compounds GaAs, InSb, are partially covalent and partially ionic.)

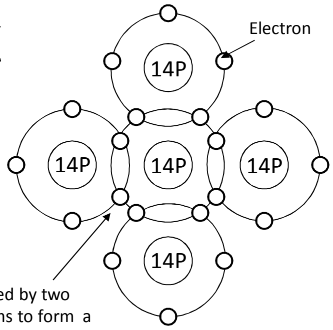
- Bond is strong (high melting point, large elastic modulus)
- Directional (from orientation of QM orbitals) → low density
- Saturable (limited number of bonds per atom) ↑
- Good insulators

Silicon

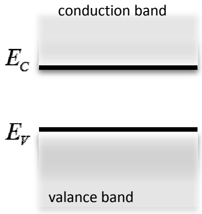


Silicon crystal

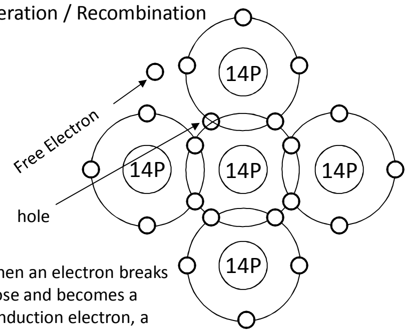
2D representation



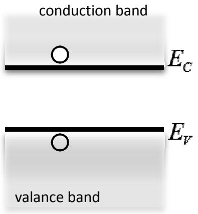
An electron shared by two neighboring atoms to form a covalent bond.
This way an atom can have a stable structure with eight valence band electrons.



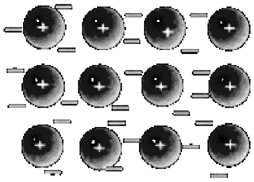
Generation / Recombination



When an electron breaks loose and becomes a conduction electron, a hole is also created.



Metallic Bonding

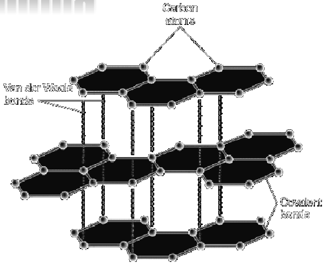


Positive ions plus gas (sea) of electrons. Think of this as the limiting case of ionic bonding in which the negative ions are electrons. (BUT electrons can't be forced to sit at lattice points from Uncertainty Principle: $\Delta p \Delta x \geq h/2$ as for electrons m is small so the zero point energy $\Delta E = \Delta p^2/2m$ is very large; the electrons would shake themselves free and are therefore delocalized)

- Bonds are non directional (high coordination number, high density, malleable and ductile)
- Variable strength
- Free electrons → high electrical conductivity, shiny

(Electric field associated with incident light makes free electrons at surface move back and forth, re-radiating the light, as a reflected beam)

Van der Waals Bonding



Even a neutral atom with a full shell, can, at a given instant, have a dipole moment (i.e. one side of the atom more positive than the other)
This instantaneous dipole will induce a dipole in a neighboring atom, and the resulting dipole-dipole interaction is the origin of the van der Waals bond. Although the original dipole time-averages to zero, the interaction does not – it is always attractive. Energy ~ $1/r^6$

- Bond is weak (→ low melting point, large expansion coefficient)
- Non directional so high coordination number BUT
- Long bond lengths (→ low density)

Examples: Solid inert gases (Argon, Neon), molecular solids (solid Oxygen)

Hydrogen Bonding

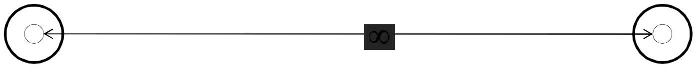
Hydrogen loses its electron and becomes positively charged particularly easily. Therefore the region of a molecule around a hydrogen atom is often quite positive, and this allows an electrostatic bond to form between it and negative parts of neighboring molecules.
Example: ice – the strength of the hydrogen bond explains the anomalously high melting point of ice

Comparing Bonds

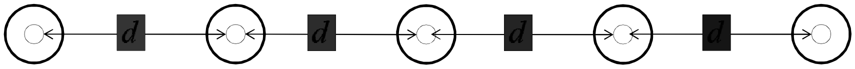
Bond	Energy (GPa)	Example of Bond
Covalent	1,000	Diamond
Ionic	30 - 100	Salt and Ceramics
Metallic	30 - 150	Metals
Hydrogen	8	Ice
Van der Vaals	2	Polythene

Energy Bands

Always simplify!
Simplest state: Isolated atom

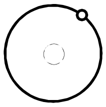


Periodic atoms:



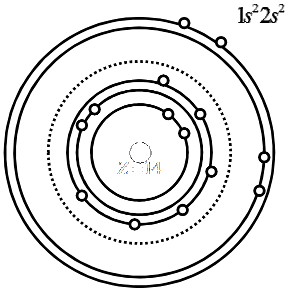
Single isolated atom:

H:



Si:

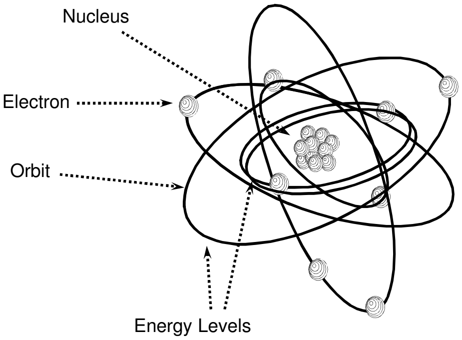
$1s^2 2s^2 2p^6 3s^2 3p^2$



Bohr Atomic Model

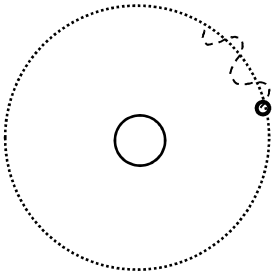
Introduced by Niels Bohr (1885 –1962) in 1913, a Dane, proposed his model of the atom while working at Cambridge University in England

Atom: a small, positively charged nucleus surrounded by electrons that travel in circular orbits around the nucleus (similar to the solar system)



passionate footballer !

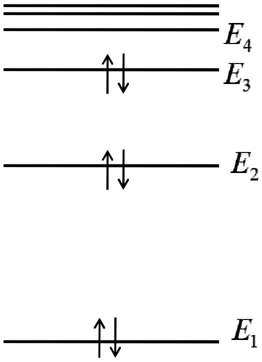
Bohr Atomic Model



wave-particle duality $\lambda = \frac{h}{p}$

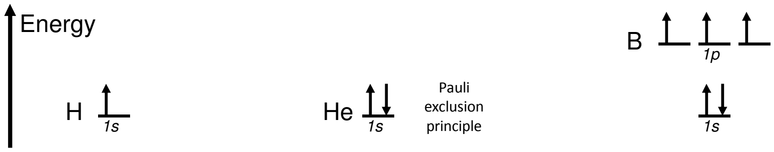
$$mvr = n\hbar$$

Energy Bands:



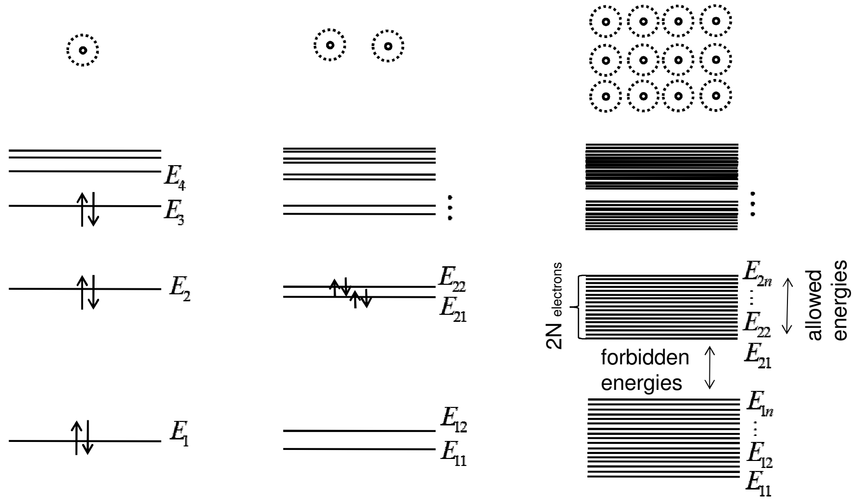
Electrons in Atoms

Electrons in an atom have particular energies (quantized energy states) depending on which orbital they are in.



Bohr Atomic Model

single atom 2 atoms N atoms

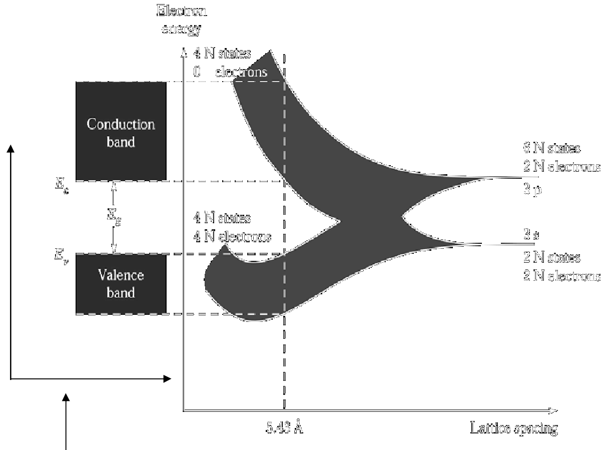


Pauli exclusion principle

Electrons in Solids

In a solid, there are so many electrons with energies very near each other that 'bands' of states develop.

Formation of energy bands as a diamond lattice crystal is formed by bringing isolated silicon atoms together.

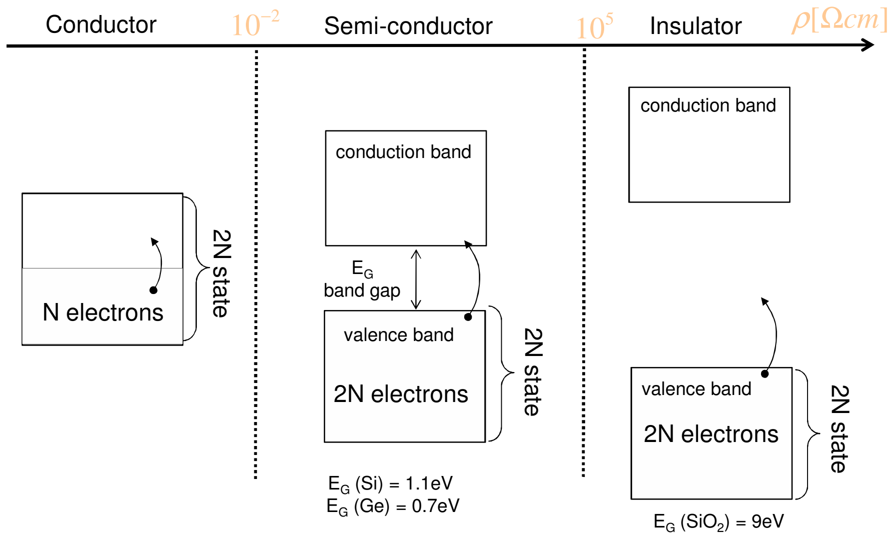


All we draw is the "band diagram"

Solid

Isolated atoms

Materials



Conductor 10^{-2} Semi-conductor 10^{5} Insulator $\rho[\Omega cm]$

N electrons

2N state

conduction band

E_G
band gap

valence band

2N electrons

2N state

E_G (Si) = 1.1eV
E_G (Ge) = 0.7eV

conduction band

valence band

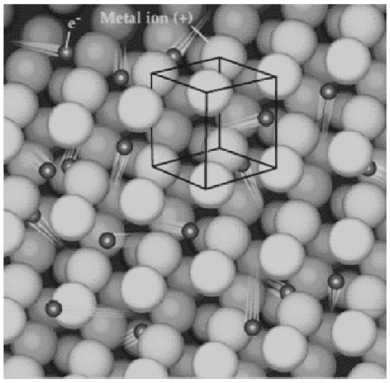
2N electrons

2N state

E_G (SiO_2) = 9eV

empty seat / filled seat

Metals

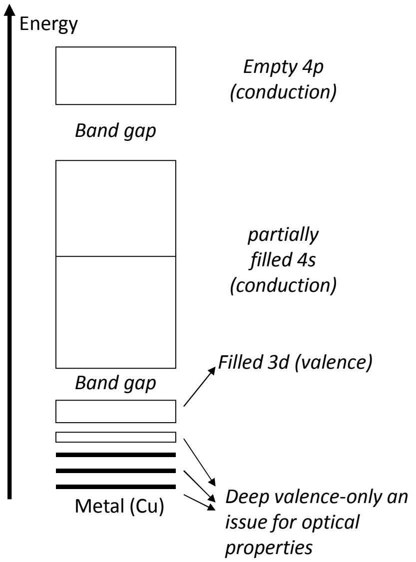


Energy Band for metals

Partially filled or empty bands are called ‘conduction bands.’

Any band that is totally filled is considered to be a “valence band.”

We usually ignore ‘deep’ valence bands.



Energy

Empty 4p (conduction)

Band gap

partially filled 4s (conduction)

Filled 3d (valence)

Band gap

Metal (Cu)

Deep valence-only an issue for optical properties

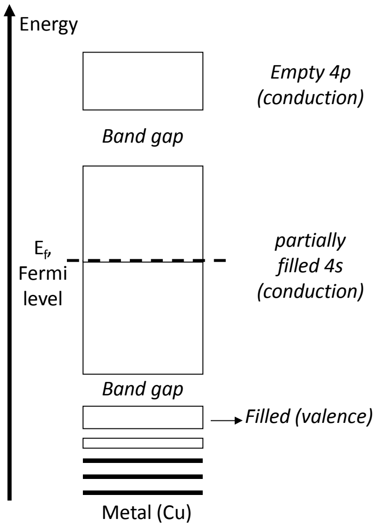
Conductivity

The free-est electron (the electron with the highest energy) defines the position of the “Fermi level.”

- Above E_f, all available electron states in the energy bands are empty
- Below E_f, they are all filled.

If there is no gap between filled and empty states, the material is conductive.

If there is a gap, the material is a semiconductor or insulator.



Energy

Empty 4p (conduction)

Band gap

E_f, Fermi level

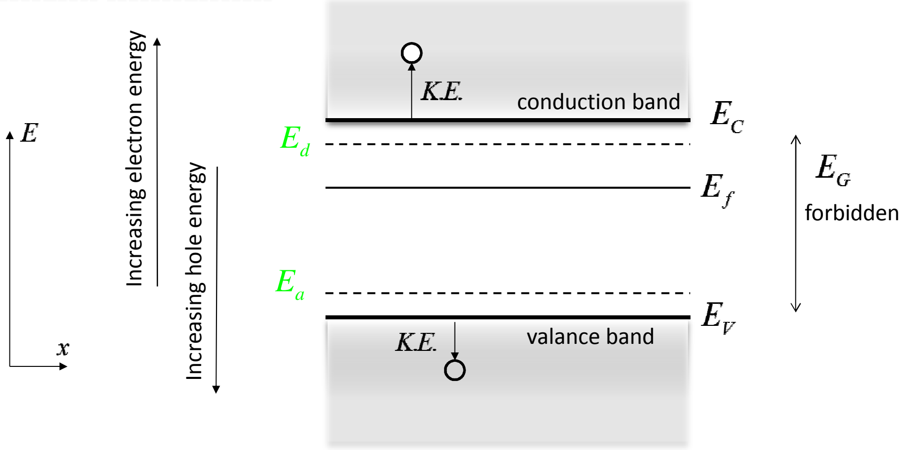
partially filled 4s (conduction)

Band gap

Filled (valence)

Metal (Cu)

Energy diagrams

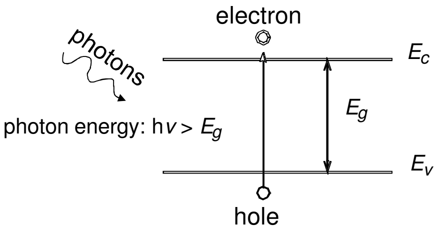


Energy band diagram shows the bottom edge of conduction band, E_c , and top edge of valence band, E_v .

E_c and E_v are separated by the **band gap energy, E_g** .

Electrons and holes tend to seek their lowest energy positions, electrons tend to fall in energy band diagram, holes float up like bubbles in water.

Measuring the Band Gap Energy by Light Absorption

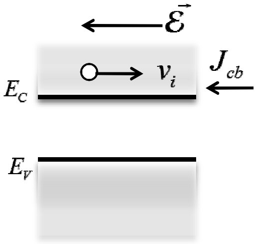


E_g can be determined from the minimum energy ($h\nu$) of photons that are absorbed by the semiconductor.

Bandgap energies of selected semiconductors

Semi-conductor	InSb	Ge	Si	GaAs	GaP	ZnSe	Diamond
Eg (eV)	0.18	0.67	1.12	1.42	2.25	2.7	6

Electron/Hole Current

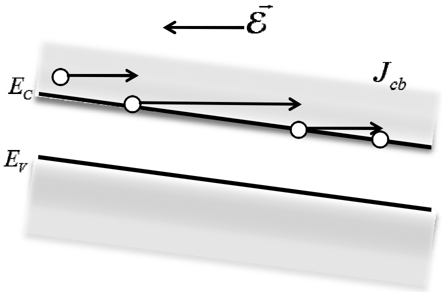


In semiconductor, electrons that are in the conduction band move by applying the electric field

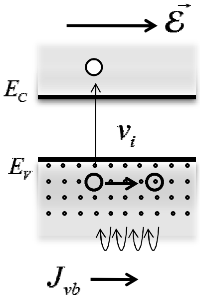
$$J_{cb} = \sum_{cb} (-q) v_i$$

As number or electrons in conduction band is much less than that in conductors hence $\rho_{SemiCond.} > \rho_{Cond.}$

More realistic picture could be:



Electron/Hole Current



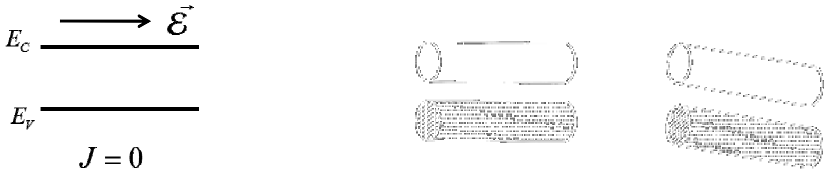
For each electron in CB there is a hole in VB (thermal excitation), Now applying an electric field will for electrons in VB to fill the empty location, hence "hole" is moving in direction of electric field!

$$J_{vb} = \sum_{vb} (-q) v_i = \sum_{filled} (-q) v_i - \sum_{empty} (-q) v_i = \sum_{empty} q v_i$$

Therefore "hole" can be considered as a positively charged particle (or an electron with negative mass!)

Analogy

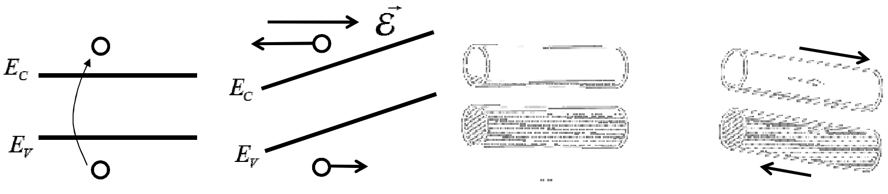
Electric field → gravitational field



$$J = 0$$

electron → droplet

hole → bubble



$$J \propto \vec{\mathcal{E}}$$

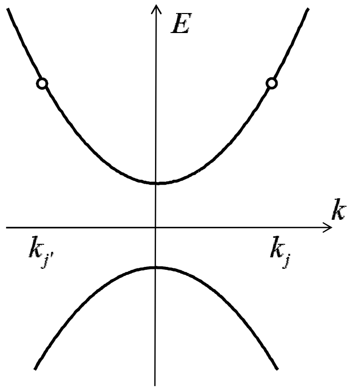
E-K diagrams

Consider a free electron with mass m,

Wave-particle duality:

$$\lambda = h/p \rightarrow p = \hbar k \qquad E = h\upsilon$$

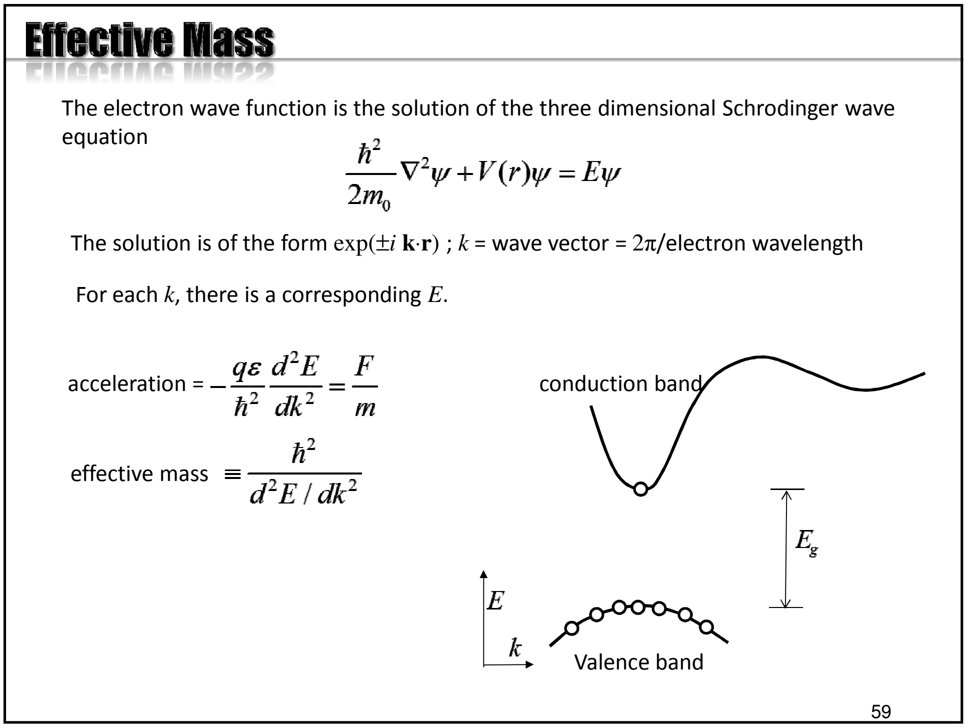
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \rightarrow E \propto k^2$$



Available states: $10^{22}/\text{cm}^3$

→ Freely moving electrons

Number of e^- & h^+ s: $10^{10}/\text{cm}^3$



Effective Mass

The electron wave function is the solution of the three dimensional Schrodinger wave equation

$$\frac{\hbar^2}{2m_0}\nabla^2\psi + V(r)\psi = E\psi$$

The solution is of the form $\exp(\pm i\,\mathbf{k}\cdot\mathbf{r})$; k = wave vector = 2π/electron wavelength

For each k, there is a corresponding E.

acceleration = $-\frac{q\varepsilon}{\hbar^2}\frac{d^2E}{dk^2} = \frac{F}{m}$

effective mass $\equiv \frac{\hbar^2}{d^2E/dk^2}$

Effective Mass

In 3-D crystals the electron acceleration will not be colinear. Thus, in general we have an effective mass tensor as

$$\frac{1}{m^*_{ij}} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

In an electric field, $\mathcal{E}$, an electron or a hole accelerates.

electrons $a = \frac{-q\mathcal{E}}{m_n}$

holes $a = \frac{-q\mathcal{E}}{m_p}$

electron and hole effective masses at 300K

for density of states calculations

	Si	Ge	GaAs
m_n/m_0	0.26	0.12	0.067
m_p/m_0	0.34	0.21	0.34

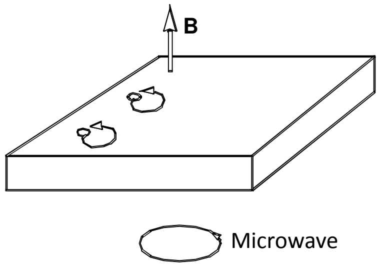
for conductivity calculations

	Si	Ge	GaAs
m_n/m_0	1.1	0.55	0.067
m_p/m_0	0.81	0.37	0.45

Measuring Effective Mass

Cyclotron Resonance Technique

Centripetal force = Lorentzian force



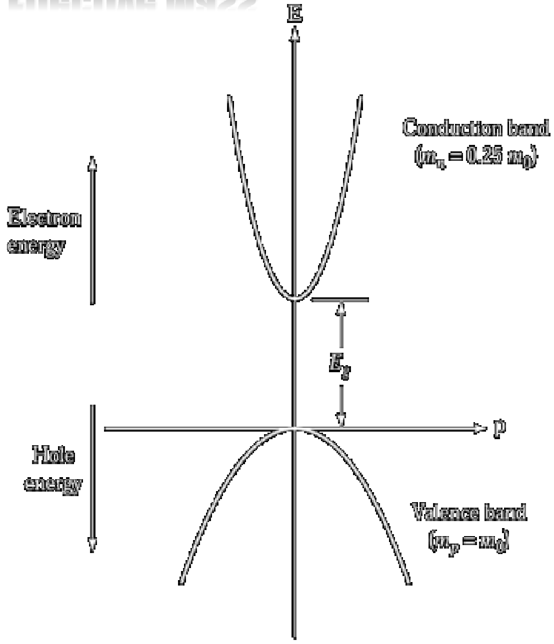
$$\frac{m_n v^2}{r} = qvB$$

$$v = \frac{qBr}{m_n}$$

$$f_{cr} = \frac{v}{2\pi r} = \frac{qB}{2\pi m_n}$$

- f_{cr} is the Cyclotron resonance frequency.
- It is independent of v and r.
- Electrons strongly absorb microwaves of that frequency.
- By measuring f_{cr}, m_n can be found.

Effective Mass

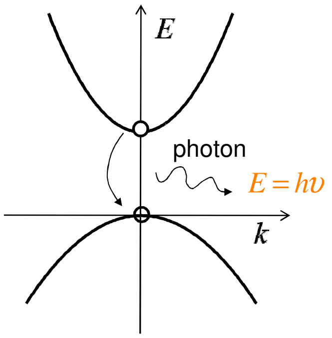


A schematic energy-momentum diagram for a special semiconductor with m_n = 0.25 m_0 and m_p = m_0.

Direct / Indirect

Direct Materials

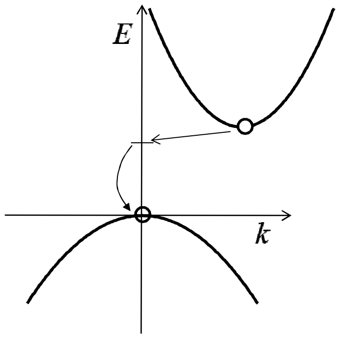
GaAs



Indirect Materials

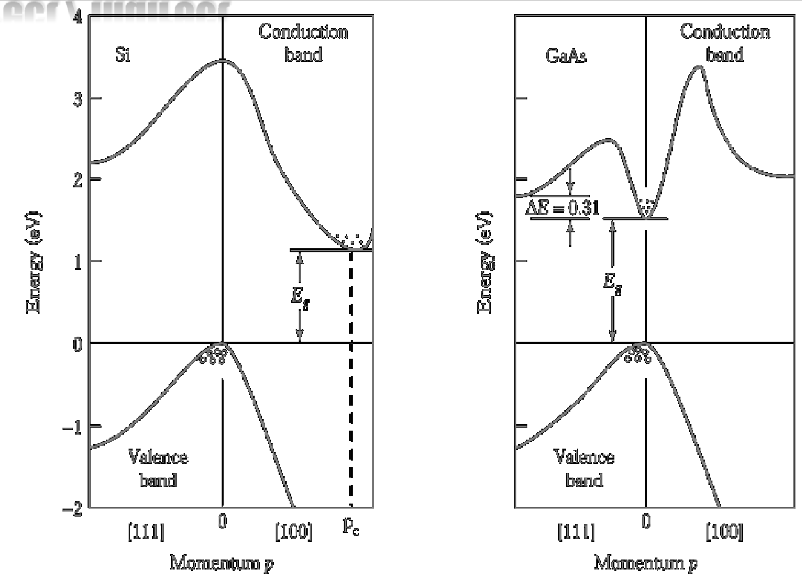
Si, Ge

Conservations of:
1. Energy
2. Momentum



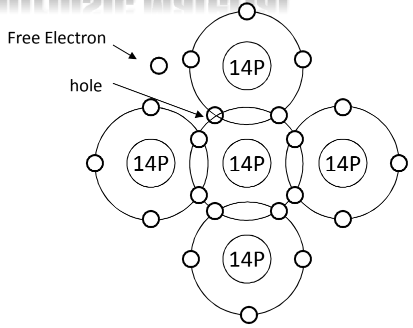
Applications: LEDs, Lasers

Direct / Indirect



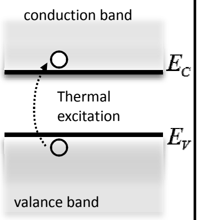
Energy band structures of Si and GaAs. Circles (º) indicate holes in the valence bands and dots (•) indicate electrons in the conduction bands.

Intrinsic Material



Intrinsic = pure

electron/hole pair is generated



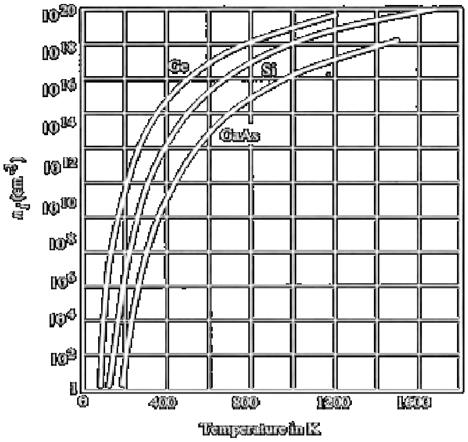
$$n = p = n_i(T)$$

n= # of e^- /cm^3
p= # of h^+ /cm^3
n_i= intrinsic carrier concentration

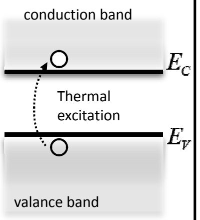
$n_{i-Si}\big|_{T=300^\circ K} = 1.5\times10^{10}\,\mathrm{cm}^{-3}$ note that totally there are $2\times10^{23}\,\mathrm{cm}^{-3}$ electrons

1 out of 10^{13} bond is broken!

Intrinsic Material



Intrinsic = pure



Energy Band Gap determines the intrinsic carrier concentration. n_i $E_{gGe} < E_{gSi} < E_{gGaAs}$

Doping

Doping means mixing a pure semiconductor with impurities to increase its electrical conductivity

Can be done in two ways:

Increasing the number of electrons by mixing pentavalent elements such as phosphorous, arsenic, antimony (means adding donor impurities)

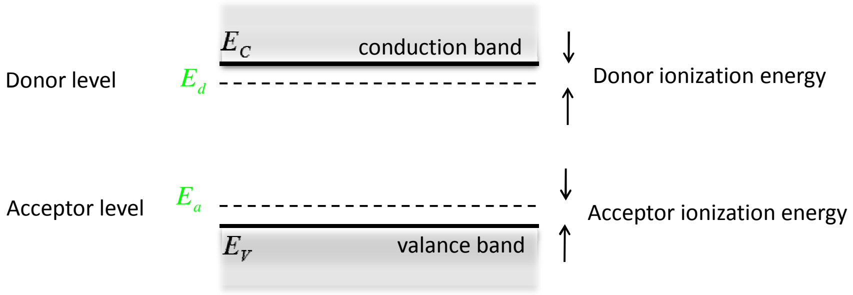
Increasing the number of holes by mixing trivalent elements such as aluminum, boron, gallium (means adding acceptor impurities)

Donors and acceptors are known as dopants.
Dopant ionization energy ~50meV (very low).

Possible dopant deactivation & defect formation

$\mathbf{N^{--}}$ **or** $\mathbf{P^{--}}$ **:** N_D or $N_A < 10^{14}\ \mathrm{cm}^{-3}$
$\mathbf{N^{-}}$ **or** $\mathbf{P^{-}}$ **:** $10^{14}\ \mathrm{cm}^{-3} < N_D$ or $N_A < 10^{16}\ \mathrm{cm}^{-3}$
N or P : $10^{16}\ \mathrm{cm}^{-3} < N_D$ or $N_A < 10^{18}\ \mathrm{cm}^{-3}$
$\mathbf{N^{+}}$ **or** $\mathbf{P^{+}}$ **:** $10^{18}\ \mathrm{cm}^{-3} < N_D$ or $N_A < 10^{20}\ \mathrm{cm}^{-3}$
$\mathbf{N^{++}}$ **or** $\mathbf{P^{++}}$ **:** N_D or $N_A > 10^{20}\ \mathrm{cm}^{-3}$

Donor and Acceptor in the Band Model



E_C conduction band

Donor level E_d

Donor ionization energy

Acceptor level E_a

Acceptor ionization energy

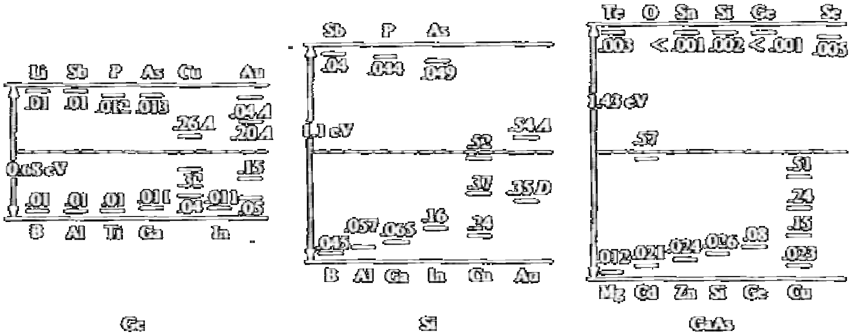
E_V valance band

$$@T = 300°K \quad KT = 26meV$$

Ionization energy of selected donors and acceptors in silicon

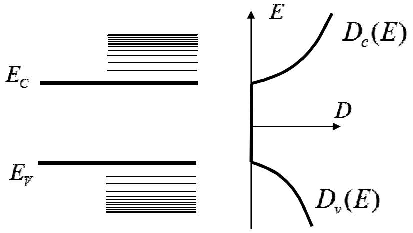
	Donors			Acceptors		
Dopant	Sb	P	As	B	Al	In
Ionization Eng Ec-Ed or Ea-Ev (meV)	39	44	54	45	57	160

Donor and Acceptor in the Band Model



Ionization energy of various impurities in Ge, Si, and GaAs at 300K.

Density of States



D(E)dE = number of states per cm3 in the energy range between E and E+dE Near the band edges:

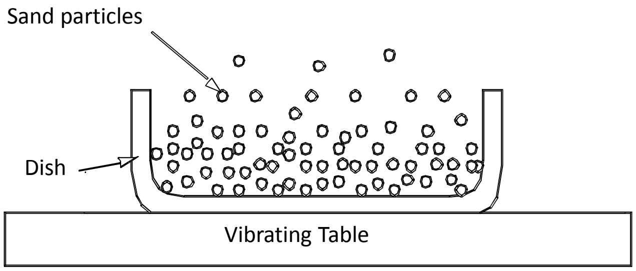
$$D_c(E) \equiv \frac{\text{number of states in } \Delta E}{\Delta E \cdot \text{volume}} \quad \left(\frac{1}{\text{eV} \cdot \text{cm}^3}\right)$$

$$g_c(E) = D_c(E) \equiv \frac{m_n\sqrt{2m_n(E - E_c)}}{\pi^2 h^3}$$

$$g_v(E) = D_v(E) \equiv \frac{m_p\sqrt{2m_p(E_v - E)}}{\pi^2 h^3}$$

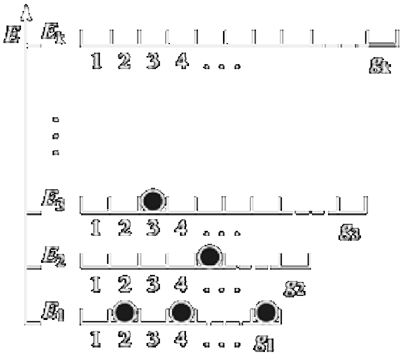
Thermal Equilibrium and the Fermi Function

An Analogy for Thermal Equilibrium



There is a certain probability for the electrons in the conduction band to occupy high-energy states under the agitation of thermal energy.

Probability of a State at E being Occupied



- There are g_1 states at E_1, g_2 states at E_2… There are N electrons, which constantly shift among all the states but the average electron energy is fixed at 3kT/2.
- There are many ways to distribute N among n_1, n_2, n_3….and satisfy the 3kT/2 condition.
- The equilibrium distribution is the distribution that maximizes the number of combinations of placing n_1 in g_1 slots, n_2 in g_2 slots…. :

$$\frac{n_i}{g_i} = \frac{1}{1+e^{(E-E_F)/kT}}$$

E_F is a constant determined by the condition $\sum_i n_i = N$

Fermi Function

Particles can be classified into 3 categories:

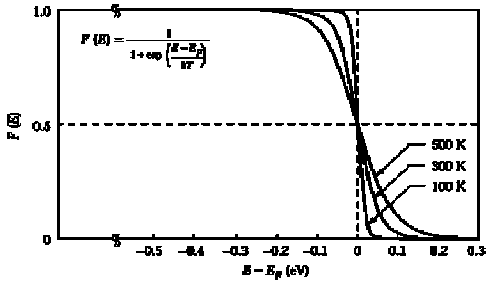
1. Classical particles	(ball)	Maxwell-Boltzmann dist.
2. Bosons	(photons)	Bose-Einstein dist.
3. Fermions(undist + Pauli Exclution)	(electrons)	Fermi-Dirac dist.

Probability that an available state at energy E is occupied:

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

E_f is called the ***Fermi energy*** or the ***Fermi level.***
There is only one Fermi level in a system at equilibrium**.**

Boltzmann constant, *k* = 8.62×10^{-5} eV/K



Fermi Function–Probability of Electron Distribution

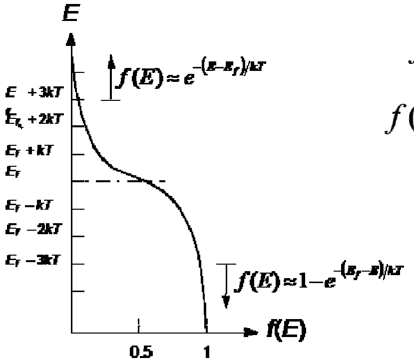
$$f(E)=\frac{1}{1+e^{(E-E_f)/kT}}$$

E_f is called the ***Fermi energy*** or the ***Fermi level.***

If we are 3kT away from the Fermi energy then we might use Boltzmann approximation:

$$f(E)\approx e^{-(E-E_f)/kT}\qquad E-E_f>>kT$$

$$f(E)\approx 1-e^{-(E_f-E)/kT}\qquad E-E_f<<-kT$$



$$-\frac{\partial f}{\partial E}\approx\delta(E-E_f)$$

Electron and Hole Concentrations

Derivation of n and p from D(E) and f(E)

Integrate n(E) over all the energies in the conduction band to obtain n

$$n = \int_{E_c}^{\text{top of conduction band}} f(E) D_c(E)\, dE$$

$$n = \frac{m_n\sqrt{2m_n}}{\pi^2 h^3} \int_{E_c}^{\infty} \sqrt{E-E_c}\, e^{-(E-E_f)/kT} dEa$$

using the Boltzmann approximation , and extending the integration limit to ∞

$$= \frac{m_n\sqrt{2m_n}}{\pi^2 h^3} e^{-(E_c-E_f)/kT} \int_{0}^{\infty} \sqrt{E-E_c}\, e^{-(E-E_c)/kT} d(E-E_c)$$

$$n = N_c e^{-(E_c-E_f)/kT} \qquad N_c \equiv 2\left[\frac{2\pi m_n kT}{h^2}\right]^{3/2}$$

N_c is called the effective density of states of the conduction band.

$$p = \int_{\text{bottom of valence band}}^{E_v} \left[1-f(E)\right] D_v(E)\, dE$$

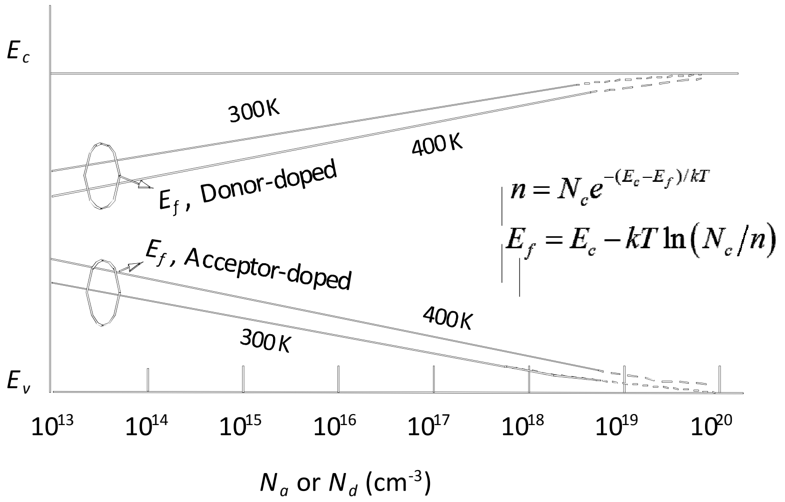
$$p = N_v e^{-(E_f-E_v)/kT} \qquad N_v \equiv 2\left[\frac{2\pi m_p kT}{h^2}\right]^{3/2}$$

N_v is called the effective density of states of the valence band.

Closer E_f to E_c the larger n , closer E_f to E_v the larger p

For Si: $N_c = 2.8\times10^{19}$ cm^{-3} , $N_v = 1.04\times10^{19}$ cm^{-3}

The Fermi Level and Carrier Concentrations



$$n = N_c e^{-(E_c-E_f)/kT}$$

$$E_f = E_c - kT\ln\left(N_c/n\right)$$

Carrier Concentrations

Multiply $n = N_c e^{-(E_c - E_f)/kT}$ and $p = N_v e^{-(E_f - E_v)/kT}$

$$np = N_c N_v e^{-(E_c - E_v)/kT} = N_c N_v e^{-E_g/kT}$$

Law of Mass Action

$$np = n_i^2$$

In an intrinsic (undoped) semiconductor, *n = p = n$_i$*.

$$n_i = \sqrt{N_c N_v}\, e^{-E_g/2kT}$$

n$_i$ is the intrinsic carrier concentration, ~10^{10} cm^{-3} for Si.

$$N_c \equiv 2\left[\frac{2\pi m_n kT}{h^2}\right]^{3/2} \qquad N_v \equiv 2\left[\frac{2\pi m_p kT}{h^2}\right]^{3/2} \qquad n_i(T) = \ldots$$

E$_i$=E$_f$ when n=p

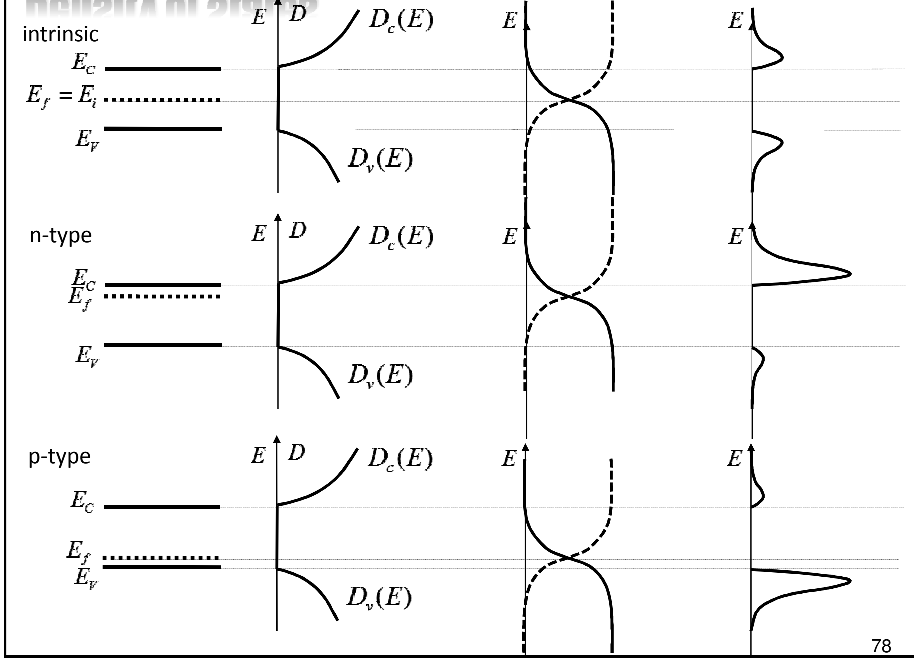
$$E_i \equiv \frac{E_c + E_v}{2} + \frac{kT}{2}\ln\left(\frac{N_v}{N_c}\right) = \frac{E_c + E_v}{2} + \frac{3kT}{4}\ln\left(\frac{m_p^*}{m_n^*}\right) \cong \frac{E_c + E_v}{2}$$

$$n = N_c e^{-(E_c - E_f)/kT} = n_i e^{(E_F - E_i)/kT}$$

$$p = N_v e^{-(E_f - E_v)/kT} = n_i e^{(E_i - E_F)/kT}$$

77

Density of States

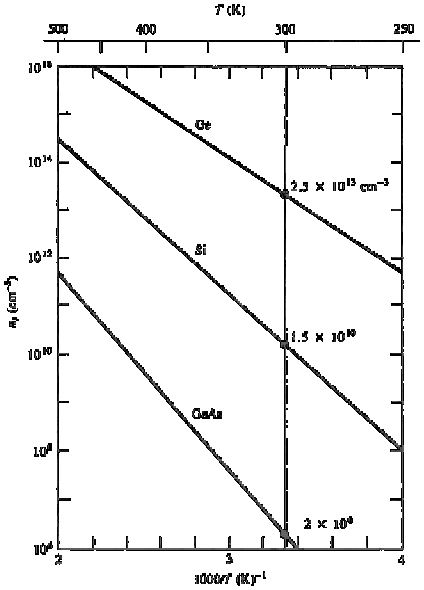


78

Ni vs. Temp

$$n_i = \sqrt{N_c N_v}\, e^{-E_g/2kT}$$

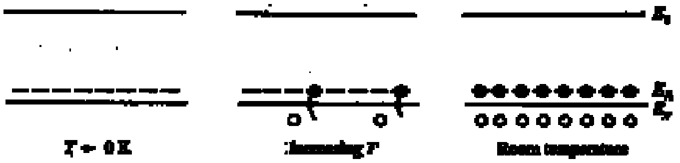
$$n_i = 2\left(\frac{2\pi KT}{h^2}\right)^{3/2} (m_n^* m_p^*)^{3/4} e^{-E_g/2kT}$$



Dopant Ionization

Donor

Acceptor

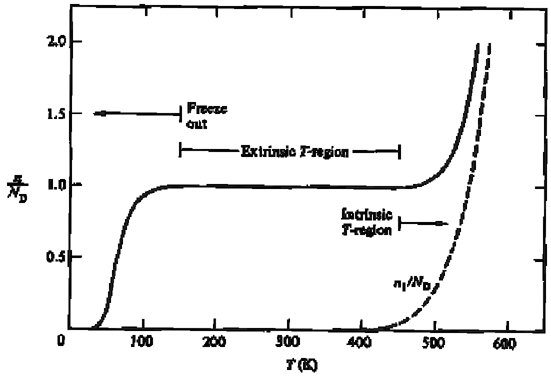


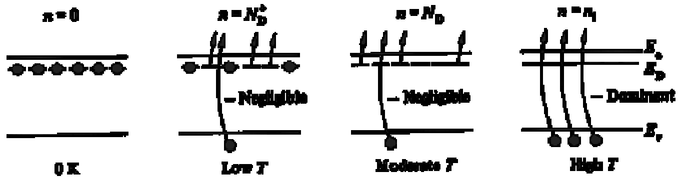
Carrier Concentration vs. Temperature

At room temperature, all the shallow dopants are ionized. (Extrinsic region)

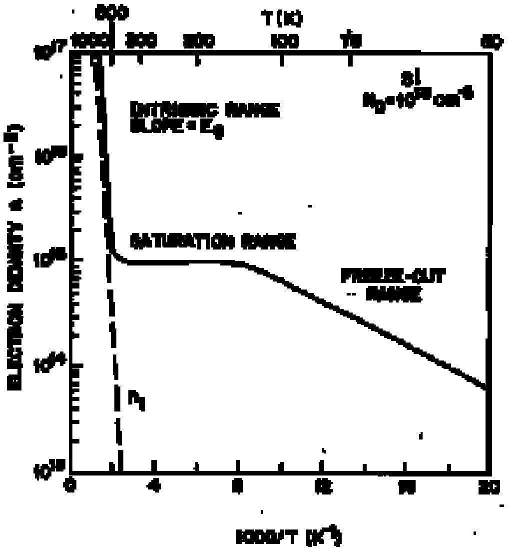
When the temperature is decreased sufficiently (~100 K), some of the dopants are not ionized. (Freeze out region)

When the temperature is increased so high that the intrinsic carrier conc. approaches the active dopant conc. (T → T_i, > 450K for Si), the semiconductor is said to enter the intrinsic region.





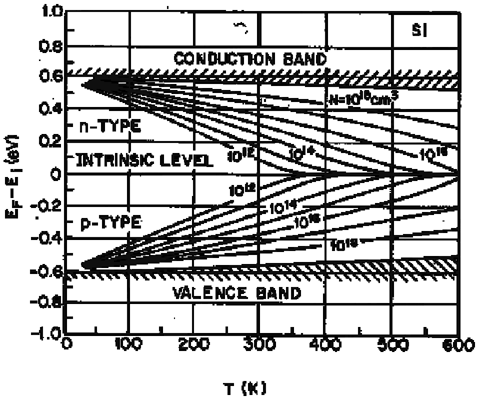
Carrier Concentration vs. Temperature



Fermi Level vs. Temperature

When the temperature is decreased, the Fermi level rises towards the donor level (N-type) and eventually gets above it.

When the temperature is increased, the Fermi level moves towards the intrinsic level.



Carrier Concentrations

Q: What is the hole concentration in an N-type semiconductor with 10^{15} cm^{-3} of donors?

Sol: n = 10^{15} cm^{-3}.

$$p = \frac{n_i^2}{n} \approx \frac{10^{20}\,\text{cm}^{-3}}{10^{15}\text{cm}^{-3}} = 10^5\,\text{cm}^{-3}$$

After increasing T by 60°C, n remains the same at 10^{15} cm^{-3} while p increases by about a factor of 2300 because $n_i^2 \propto e^{-E_g/kT}$.

Q: What is n if p = 10^{17}cm^{-3} in a P-type silicon wafer?

Sol:

$$n = \frac{n_i^2}{p} \approx \frac{10^{20}\,\text{cm}^{-3}}{10^{17}\text{cm}^{-3}} = 10^3\,\text{cm}^{-3}$$

Dopant Ionization

Consider a phosphorus-doped Si sample at 300K with $N_D = 10^{17}$ cm^{-3}. What fraction of the donors are not ionized?

Answer: Suppose **all** of the donor atoms are ionized.

Then $E_F = E_c - kT\ln\left(N_c/n\right) = E_c - 150meV$

$$\frac{N_D^+}{N_D} = \frac{1}{1+g_D e^{(E_F-E_D)/kT}} \qquad \frac{N_A^-}{N_A} = \frac{1}{1+g_A e^{(E_F-E_D)/kT}}$$

$$g_D = 2 \qquad g_A = 4$$

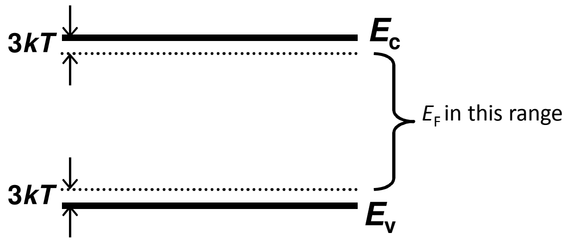
Probability of non-ionization ≅ $\frac{1}{1+\frac{1}{2}e^{(E_D-E_F)/kT}}$

$$= \frac{1}{1+\frac{1}{2}e^{(150meV-45meV)/26meV}} = 0.034$$

Nondegenerately Doped Semiconductor

Recall that the expressions for *n* and *p* were derived using the Boltzmann approximation, *i.e.* we assumed

$$E_v + 3kT \le E_F \le E_c - 3kT$$



The semiconductor is said to be ***nondegenerately doped*** in this case.

Degenerately Doped Semiconductor

If a semiconductor is very heavily doped, the Boltzmann approximation is not valid.

In Si at T=300K: E_c-E_F < $3kT$ if $N_D > 1.6\text{x}10^{18}$ cm^{-3}

E_F-E_v < $3kT$ if $N_A > 9.1\text{x}10^{17}$ cm^{-3}

The semiconductor is said to be ***degenerately doped*** in this case.

<u>Terminology</u>:

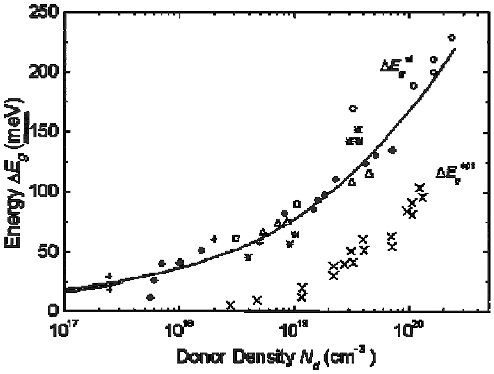
"n+" → degenerately n-type doped. $E_F \cong E_c$

"p+" → degenerately p-type doped. $E_F \cong E_v$

Band Gap Narrowing

If the dopant concentration is a significant fraction of the silicon atomic density, the energy-band structure is perturbed → the band gap is reduced by ΔE_G :

$$\Delta E_G \cong 3.5\times10^{-8} N^{1/3}\sqrt{\frac{300}{T}}$$



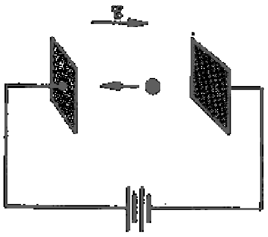
$N = 10^{18}$ cm^{-3}: ΔE_G = 35 meV
$N = 10^{19}$ cm^{-3}: ΔE_G = 75 meV

Mobile Charge Carriers in Semiconductors

- Three primary types of carrier action occur inside a semiconductor:
  - Drift: charged particle motion under the influence of an electric field.
  - Diffusion: particle motion due to concentration gradient or temperature gradient.
  - Recombination-generation (R-G)

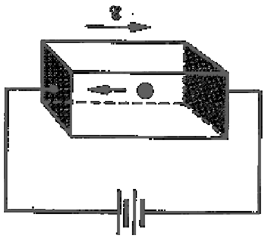
Electrons as Moving Particles

In vacuum



$$\mathbf{F} = (-q)\mathcal{E} = m_0\mathbf{a}$$

In semiconductor



$$\mathbf{F} = (-q)\mathcal{E} = m_n^*\mathbf{a}$$

where m_n^* is the electron effective mass

Thermal velocity

We saw that

In an electric field, $\mathcal{E}$, an electron or a hole accelerates.

electrons $a = \frac{-q\mathcal{E}}{m_n^*}$

holes $a = \frac{-q\mathcal{E}}{m_p^*}$

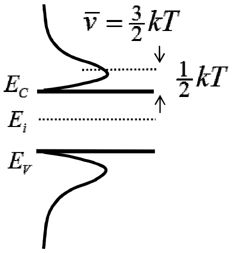
electron and hole effective masses

	Si	Ge	GaAs
m^*_n/m_0	0.26	0.12	0.068
m^*_p/m_0	0.39	0.3	0.5

Average electron kinetic energy $= \frac{3}{2}kT = \frac{1}{2}m_n^* v_{th}^2$

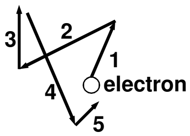
$$v_{th} = \sqrt{\frac{3kT}{m_n^*}} = \sqrt{\frac{3 \times 0.026\text{eV} \times (1.6 \times 10^{-19}\,\text{J/eV})}{0.26 \times 9.1 \times 10^{-31}\text{kg}}}$$

$$= 2.3 \times 10^5\,\text{m/s} = 2.3 \times 10^7\,\text{cm/s}$$



Carrier Scattering

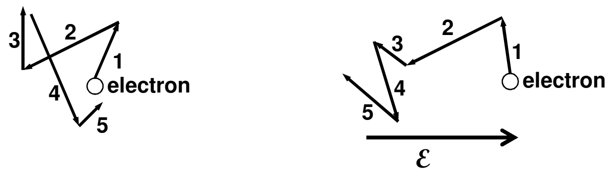
Mobile electrons and atoms in the Si lattice are always in random thermal motion.
Electrons make frequent collisions with the vibrating atoms called “lattice scattering” or “phonon scattering” (increases with increasing temperature)
Average velocity of thermal motion for electrons: ~10^7 cm/s @ 300K



Other scattering mechanisms:
deflection by ionized impurity atoms
deflection due to Coulombic force between carriers (carrier-carrier scattering)
only significant at high carrier concentrations
The net current in any direction is zero, if no electric field is applied.

Carrier Drift

When an electric field (e.g. due to an externally applied voltage) is applied to a semiconductor, mobile charge carriers will be accelerated by the electrostatic force. This force superimposes on the random motion of electrons:



Electrons *drift* in the direction opposite to the electric field

→ current flows

Because of scattering, electrons in a semiconductor do not achieve constant acceleration. However, they can be viewed as quasi-classical particles moving at a constant average *drift velocity* v_d

Carrier Mobility

With every collision, the electron loses momentum $m_n^* v_d$

Between collisions, the electron gains momentum $(-q)\mathcal{E}\bar{\tau}$

$\bar{\tau}$ is the average time between electron scattering events
mean time between collisions

In steady state

$$m_n^* v_d = (-q)\mathcal{E}\bar{\tau}$$

$$|v_d| = q\mathcal{E}\bar{\tau}/m_n^* = \mu_n \mathcal{E}$$

$$\mu_n \equiv \frac{q\bar{\tau}_n}{m_n^*}$$ is the electron mobility

Similarly for holes $$\mu_p \equiv \frac{q\bar{\tau}_p}{m_p^*}$$ is the hole mobility

Electron and hole mobilities of selected intrinsic semiconductors (T=300K)

Mean Free Path

Average distance traveled between collisions is called mean free path

$$\lambda = v_{th}\overline{\tau}$$

This is an important length, structures at the order or smaller that m.f.p. show different performance.

Mechanisms of Carrier Scattering

Dominant scattering mechanisms:

Phonon scattering (lattice scattering) | Impurity (dopant) ion scattering

Phonon scattering mobility decreases when T increases:

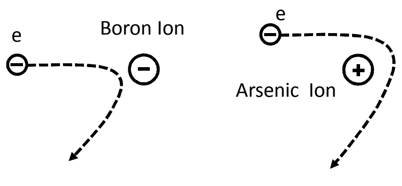
$$\mu_{phonon} \propto \tau_{phonon} \propto \frac{1}{\text{phonon density} \times \text{carrier thermal velocity}}$$

$$\propto \frac{1}{T \times T^{1/2}} \propto T^{-3/2}$$

$$\uparrow$$

$$v_{th} \propto \sqrt{T}$$

There is less change in the electron's direction of travel if the electron zips by the ion at a higher speed.



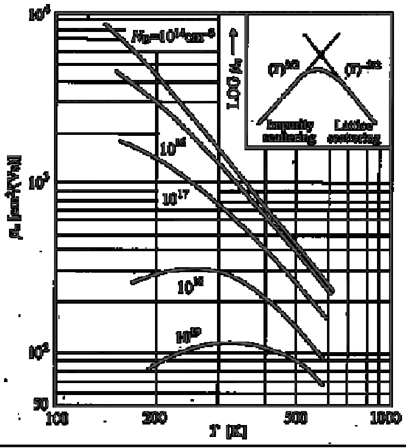
$$\mu_{impurity} \propto \frac{v_{th}^3}{N_A + N_D} \propto \frac{T^{3/2}}{N_A + N_D}$$

Matthiessen's Rule

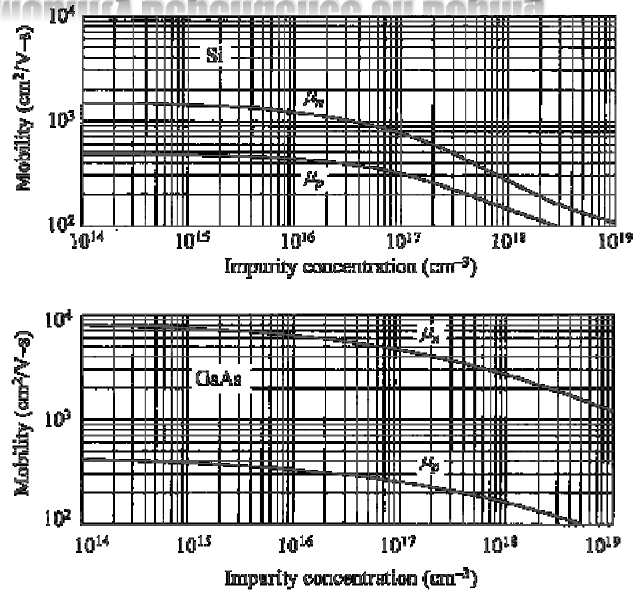
The probability that a carrier will be scattered by mechanism i within a time period dt is dt/τ_i , where τ_i is the mean time between scattering events due to mechanism i. Hence,The probability that a carrier will be scattered within a time period dt is $\sum dt/\tau_i$

$$\frac{1}{\tau}=\frac{1}{\tau_{phonon}}+\frac{1}{\tau_{impurity}}\Rightarrow\frac{1}{\mu}=\frac{1}{\mu_{phonon}}+\frac{1}{\mu_{impurity}}$$

Temperature Effect on Mobility



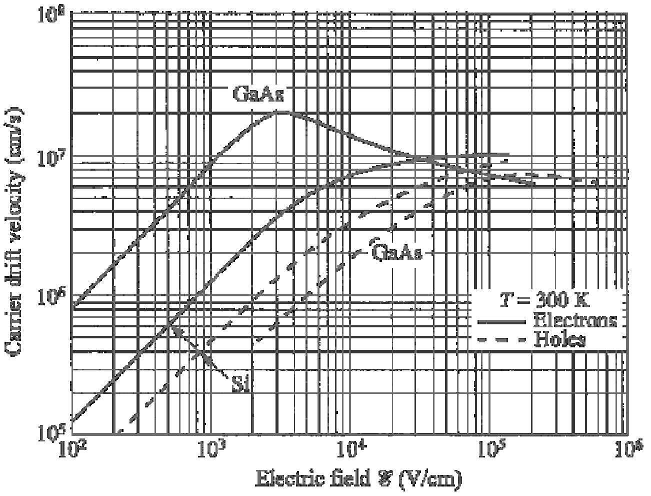
Mobility Dependence on Doping



$$\frac{1}{\mu}=\frac{1}{\mu_{phonon}}+\frac{1}{\mu_{impurity}}$$

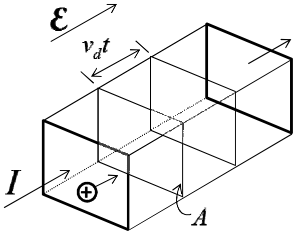
Total Doping Concentration $N_A + N_D$ (cm^{-3})

Velocity Saturation



Carrier velocity vs. electric field

Drift Current



volume from which all holes cross plane in time t = $v_d tA$

# of holes crossing plane in time t = $pv_d tA$

charge crossing plane in time t = $qpv_d tA$

charge crossing plane per unit time = hole current = $qpv_d A$

→ Hole current per unit area = $J_p = I/A = qpv_d$

$$J_{n,drift} = -qnv = qn\mu_n \mathcal{E}$$

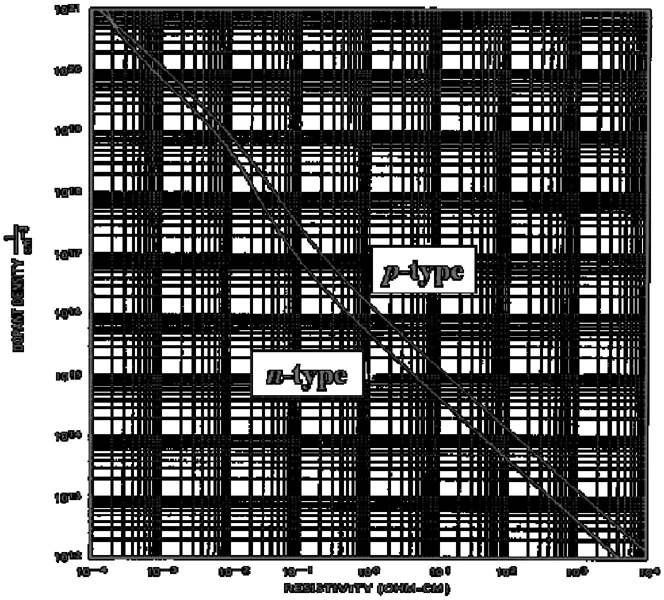
$$J_{p,drift} = qnv = qn\mu_p \mathcal{E}$$

$$J_{drift} = J_{n,drift} + J_{p,drift} = \sigma \mathcal{E} = \left(qn\mu_n + qn\mu_p\right)\mathcal{E}$$

Conductivity of a semiconductor is $\sigma \equiv qn\mu_n + qp\mu_p$

Resistivity $\rho \equiv 1/\sigma$ (Unit: ohm-cm)

Resistivity Dependence on Doping



For n-type material:

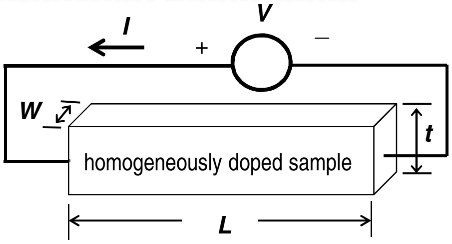
$$\rho \cong \frac{1}{qn\mu_n}$$

For p-type material:

$$\rho \cong \frac{1}{qp\mu_p}$$

Note: This plot does not apply for compensated material!

Electrical Resistance



Resistance (Ohms)

$$\sigma = \frac{1}{\rho} = \frac{J}{\mathcal{E}} = \frac{I/Wt}{V/L} \rightarrow R \equiv \frac{V}{I} = \rho\frac{L}{Wt}$$

Q: Consider a Si sample doped with $10^{16}/cm^3$ Boron. What is its resistivity?

A: $N_A = 10^{16}/cm^3$, $N_D = 0$ ($N_A >> N_D$ hence p-type)
→ $p \approx 10^{16}/cm^3$ and $n \approx 10^4/cm^3$

$$\rho = \frac{1}{qn\mu_n + qp\mu_p} \cong \frac{1}{qp\mu_p}$$

$$= \left[(1.6\times10^{-19})(10^{16})(450)\right]^{-1} = 1.4\ \Omega\text{cm}$$

Q: Consider the same Si sample, doped additionally with $10^{17}/cm^3$ Arsenic. What is its resistivity?

A: $N_A = 10^{16}/cm^3$, $N_D = 10^{17}/cm^3$ ($N_D >> N_A$ hence n-type)
→ $n \approx 9\times10^{16}/cm^3$ and $p \approx 1.1 \times 10^3/cm^3$

$$\rho = \frac{1}{qn\mu_n + qp\mu_p} \cong \frac{1}{qp\mu_n}$$

$$= \left[(1.6\times10^{-19})(9\times10^{16})(600)\right]^{-1} = 0.12\ \Omega\text{cm}$$

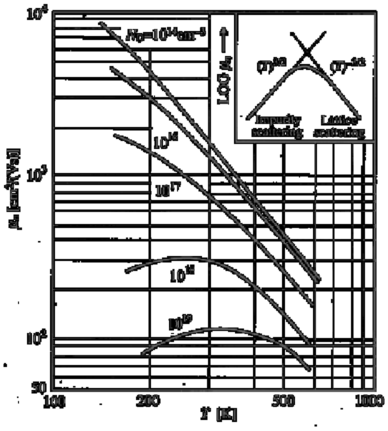
Electrical Resistance

Q: Consider a Si sample doped with 10^{17}cm^{-3} As. How will its resistivity change when the temperature is increased from T=300K to T=400K?

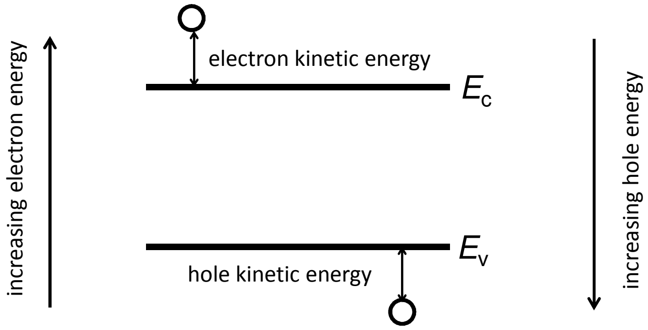
A: The temperature dependent factor in σ (and therefore ρ) is μ_n.

From the mobility *vs.* temperature curve for 10^{17}cm^{-3}, we find that μ_n decreases from 770 at 300K to 400 at 400K. As a result, ρ **increases** by

$$\frac{770}{400} = 1.93$$



Potential vs. Kinetic Energy



electron kinetic energy

E_c

E_v

hole kinetic energy

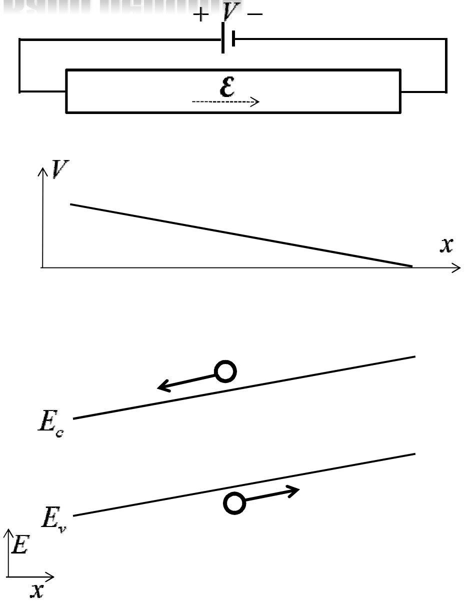
increasing electron energy

increasing hole energy

E_c represents the electron potential energy:

$$\text{P.E.} = E_c - E_{\text{reference}}$$

Band bending



The potential energy of a particle with charge -q is related to the electrostatic potential V(x):

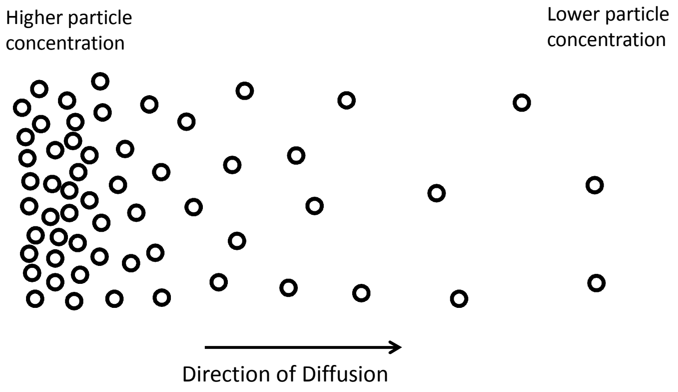
$$\text{P.E.} = -qV \qquad V = \frac{1}{q}(E_{\text{reference}} - E_{\text{c}})$$

$$\mathcal{E} = -\frac{dV}{dx} = \frac{1}{q}\frac{dE_{\text{c}}}{dx}$$

Variation of Ec with position is called "band bending."

Diffusion

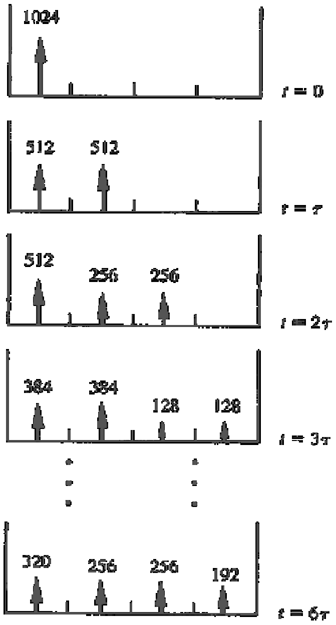
Particles diffuse from regions of higher concentration to regions of lower concentration region, due to random thermal motion



1-D Diffusion Example

Thermal motion causes particles to move into an adjacent compartment every t seconds.

Each particle has an equal probability of jumping to the left and to the right.

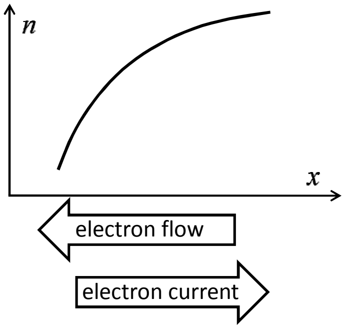


Diffusion Current

$$J_{\mathrm{N,diff}} = qD_N \frac{dn}{dx}$$

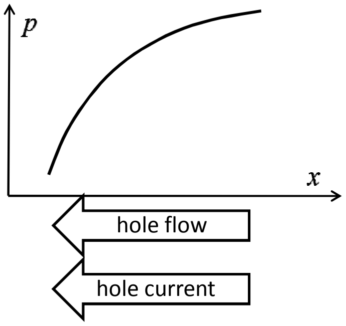
D is the diffusion constant, or diffusivity.

$$J_{\mathrm{P,diff}} = -qD_P \frac{dp}{dx}$$



electron flow

electron current



hole flow

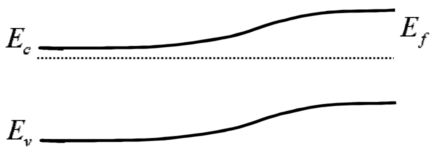
hole current

$$J = J_N + J_{\mathrm{P}}$$

$$J_N = J_{\mathrm{N,drif}} + J_{\mathrm{N,diff}} = qn\mu_n\mathcal{E} + qD_n \frac{dn}{dx} \qquad J_P = J_{\mathrm{P,drif}} + J_{\mathrm{P,diff}} = qp\mu_p\mathcal{E} + qD_p \frac{dp}{dx}$$

Non-Uniformly-Doped Semiconductor

The position of E_F relative to the band edges is determined by the carrier concentrations, which is determined by the dopant concentrations.



In equilibrium, E_F is constant; therefore, the band energies vary with position:

In equilibrium, there is no net flow of electrons or holes

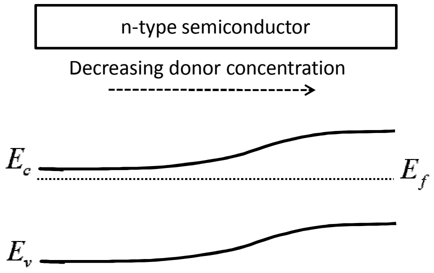
$J_N = 0$ and $J_P = 0$

The drift and diffusion current components must balance each other exactly. (A built-in electric field exists, such that the drift current exactly cancels out the diffusion current due to the concentration gradient.)

$$J_N = qn\mu_n\mathcal{E} + qD_n\frac{dn}{dx}$$

Einstein Relationship

Consider a piece of a non-uniformly doped semiconductor:



$$n = N_c e^{-(E_c-E_F)/kT}$$

$$\frac{dn}{dx} = -\frac{N_c}{kT}e^{-(E_c-E_F)/kT}\frac{dE_c}{dx}$$

$$= -\frac{n}{kT}\frac{dE_c}{dx} = -\frac{n}{kT}q\mathcal{E}$$

Under equilibrium conditions, $J_N = 0$ and $J_P = 0$

$$J_N = qn\mu_n\mathcal{E} + qD_n\frac{dn}{dx} = 0 \;= qn\mu_n\mathcal{E} - qD_n\frac{n}{kT}q\mathcal{E} \quad \rightarrow D_n = \frac{kT}{q}\mu_n$$

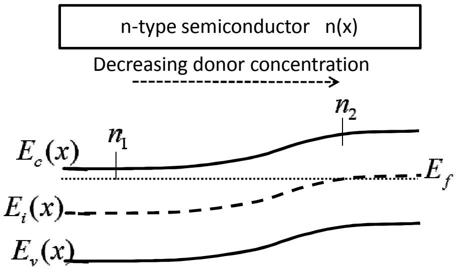
Similarly: $\rightarrow D_p = \frac{kT}{q}\mu_p$

Einstein Relationship

Note: The Einstein relationship is valid for a non-degenerate semiconductor, even under non-equilibrium conditions

Potential Difference due to n(x), p(x)

Consider a piece of a non-uniformly doped semiconductor:


n-type semiconductor n(x)

Decreasing donor concentration

$$n = N_c E_F - E_{i1} = kT\ln\left(\frac{n_1}{n_i}\right)$$

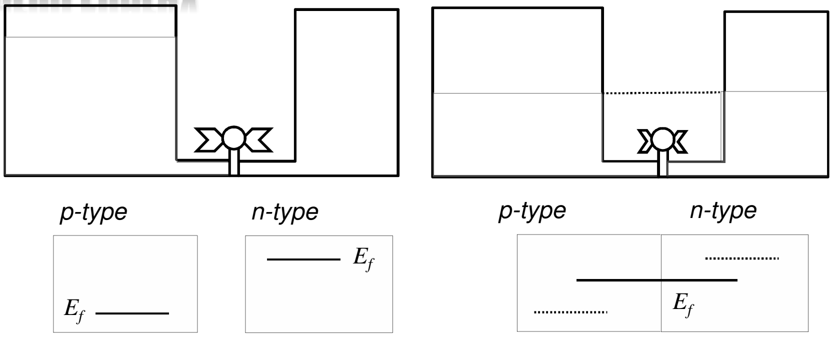
$$\rightarrow E_{i1} = E_F - kT\ln\left(\frac{n_1}{n_i}\right)$$

Similarly: $$E_{i2} = E_F - kT\ln\left(\frac{n_2}{n_i}\right)$$

Therefore: $$E_{i1} - E_{i2} = kT\left[\ln\left(\frac{n_2}{n_i}\right) - \ln\left(\frac{n_1}{n_i}\right)\right] = kT\ln\left(\frac{n_2}{n_1}\right)$$

$$V_2 - V_1 = \frac{1}{q}\left(E_{i1} - E_{i2}\right) = \frac{kT}{q}\ln\left(\frac{n_2}{n_1}\right)$$

Fermi Energy



Density of state: $D_1(E)$ $D_2(E)$

Fermi dist.: $f_1(E)$ $f_2(E)$

$$D_1(E)f_1(E)\cdot\left[D_2(E)(1-f_2(E))\right]$$

$$D_2(E)f_2(E)\cdot\left[D_1(E)(1-f_1(E))\right]$$

$$D_1(E)f_1(E)\cdot\left[D_2(E)(1-f_2(E))\right] = D_2(E)f_2(E)\cdot\left[D_1(E)(1-f_1(E))\right]$$
$$\rightarrow f_1(E) = f_2(E) \rightarrow E_{F1} = E_{F2}$$

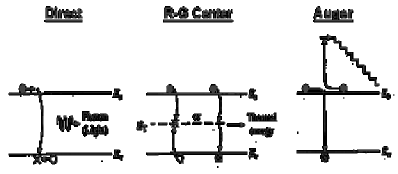
Non-Equilibrium Processes

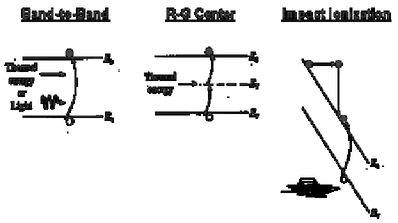
Whenever the thermal-equilibrium condition of a semiconductor system is disturbed $pn \neq n_i^2$ processes exist to restore the system to equilibrium

Generation and recombination processes act to change the carrier concentrations, and thereby indirectly affect current flow

Recombination mechanisms $np > n_i^2$

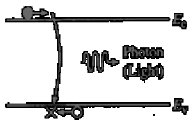
Generation mechanisms $np < n_i^2$



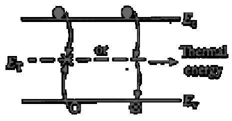


Recombination in Si is primarily via R-G centers

Recombination Mechanisms

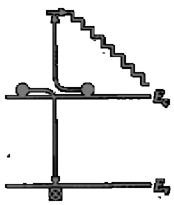


Direct or Band to Band
Basis for light emission devices
Photon (single particle of light) or multiple phonons (single quantum of lattice vibration – equivalent to saying thermal energy)



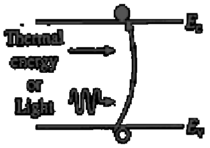
Energy loss can result in a Photon but more often multiple Phonons

R-G Center
Also known as Schockley-Read-Hall (SRH) recombination
Photon (single particle of light) or multiple phonons (single quantum of lattice vibration – equivalent to saying thermal energy)
Note: Trap level, Two steps: 1st Carrier is trapped at a defect/impurity, 2nd Carrier (opposite type) is attracted to the RG center and annihilates the 1st carrier

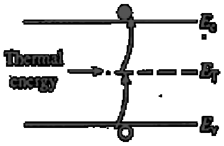


Auger
Requires 3 particles, Two steps:
1st carrier and 2nd carrier of the same type collide instantly annihilating the electron hole pair (1st and 3rd carrier).
The energy lost in he annihilation process is given o the 2nd carrier.
2nd carrier gives off a series of phonons until it's energy returns to equilibrium energy (E~Ec)

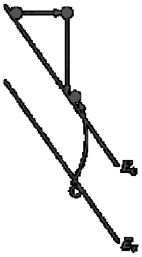
Generation Mechanisms



Direct of Band to Band
Does not have to be a direct bandgap material
Mechanism that results in ni
Basis for light absorption devices such as semiconductor photodetectors, solar cells, etc.



R-G Center
Two steps:
A bonding electron is trapped at an unintentional defect/impurity generating a hole in the valence band
This trapped electron is then promoted to the conduction band resulting ina new electron-hole pair
Almost always detrimental to electronic devices



Impact Ionization
Requires 3 particles and typically high electric fields
1st carrier is accelerated by high electric fields
Collides with a lattice atom
Knocks out a bonding electron
Creates an electron hole pair
What is it called when this process repeats and what device is it useful for?

Low-Level Injection

Excess Carrier Concentrations:

equilibrium values

$$\Delta n \equiv n - n_0$$
$$\Delta p \equiv p - p_0$$

Charge neutrality condition: $\Delta n = \Delta p$

Low-Level Injection: Often the disturbance from equilibrium is small, such that the majority-carrier concentration is not affected significantly:

For an n-type material $|\Delta n| = |\Delta p| << n_0 \quad \text{so} \quad n \cong n_0$

For an p-type material $|\Delta n| = |\Delta p| << p_0 \quad \text{so} \quad p \cong p_0$

However, the minority carrier concentration can be significantly affected

Indirect Recombination Rate

Suppose excess carriers are introduced into an n-type Si sample (e.g. by temporarily shining light onto it) at time t = 0. How does p vary with time t > 0?

1. Consider the rate of hole recombination via traps:

$$\left.\frac{\partial p}{\partial t}\right|_R = -c_p N_T p$$

c_p = capture coeficient

N_T = # of traps

2. Under low-level injection conditions, the hole generation rate is not significantly affected:

$$\left.\frac{\partial p}{\partial t}\right|_G \cong \left.\frac{\partial p}{\partial t}\right|_{G-equilibrium} = -\left.\frac{\partial p}{\partial t}\right|_{R-equilibrium} = c_p N_T p_0$$

3. The net rate of change in p is therefore

$$\left.\frac{\partial p}{\partial t}\right|_{R-G} = \left.\frac{\partial p}{\partial t}\right|_R + \left.\frac{\partial p}{\partial t}\right|_G = -c_p N_T p + c_p N_T p_0$$

$$\left.\frac{\partial p}{\partial t}\right|_{R-G} = -c_p N_T (p - p_0) \equiv -\frac{\Delta p}{\tau_p} \quad \text{where} \quad \tau_p \equiv \frac{1}{c_p N_T}$$

Relaxation to Equilibrium State

Consider a semiconductor with no current flow in which thermal equilibrium is disturbed by the sudden creation of excess holes and electrons. The system will relax back to the equilibrium state via the R-G mechanism:

for electrons in p-type material: $\frac{\partial n}{\partial t} = -\frac{\Delta n}{\tau_n}$

for holes in n-type material: $\frac{\partial p}{\partial t} = -\frac{\Delta p}{\tau_p}$

$$\tau_p \equiv \frac{1}{c_p N_T} \qquad \tau_n \equiv \frac{1}{c_n N_T}$$

The minority carrier lifetime τ is the average time an excess minority carrier "survives" in a sea of majority carriers.

τ ranges from 1 ns to 1 ms in Si and depends on the density of metallic impurities (contaminants) such as Au and Pt, and the density of crystalline defects. These deep traps capture electrons or holes to facilitate recombination and are called recombination-generation centers.

Example: Photoconductor

Consider a sample of Si doped with 10^{16} cm^{-3} boron, with recombination lifetime 1μs. It is exposed continuously to light, such that electron-hole pairs are generated throughout the sample at the rate of 10^{20} per cm^3 per second, *i.e.* the **generation rate G_L** = 10^{20}/cm^3/s

1. What are p_0 and n_0?

$$p_0 = 10^{16} cm^{-3} \qquad n_0 = 10^4 cm^{-3}$$

2. What are Δn and Δp?

$$G_L = \Delta n / \tau_n = 10^{20}$$
$$\Delta n = \Delta p = G_L \tau = 10^{20} \times 10^{-6} = 10^{14} cm^{-3}$$

3. What are p and n?

$$p = p_0 + \Delta p = 10^{16} + 10^{14} \approx 10^{16} cm^{-3}$$
$$n = n_0 + \Delta n = 10^4 + 10^{14} \approx 10^{14} cm^{-3}$$

4. What is the np product?

$$np = 10^{30} cm^{-3} >> n_i^2$$

Net Recombination Rate (General Case)

For arbitrary injection levels and both carrier types in a non-degenerate semiconductor, the net rate of carrier recombination is:

$$-\frac{\partial \Delta n}{\partial t} = -\frac{\partial \Delta p}{\partial t} = \frac{pn - n_i^2}{\tau_p (n + n_1) + \tau_n (p + p_1)}$$
$$\text{where } n_1 \equiv n_i e^{(E_T - E_i)/kT} \text{ and } p_1 \equiv n_i e^{(E_i - E_T)/kT}$$

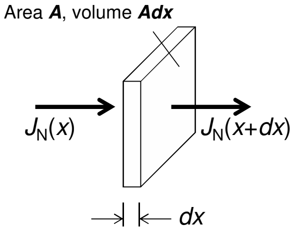
For low level injection:

for electrons in p-type material: $\frac{\partial n}{\partial t} = -\frac{\Delta n}{\tau_n}$

for holes in n-type material: $\frac{\partial p}{\partial t} = -\frac{\Delta p}{\tau_p}$

Derivation of Continuity Equation

Consider carrier-flux into/out-of an infinitesimal volume:



$$Adx\left(\frac{\partial n}{\partial t}\right) = -\frac{1}{q}\left[J_N(x)A - J_N(x+dx)A\right] - \frac{\Delta n}{\tau_n}Adx$$

$$J_N(x+dx) = J_N(x) + \frac{\partial J_N(x)}{\partial x}dx$$

$$\Rightarrow \quad \frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_N(x)}{\partial x} - \frac{\Delta n}{\tau_n}$$

Continuity Equation

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_N(x)}{\partial x} - \frac{\Delta n}{\tau_n} + G_L$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_P(x)}{\partial x} - \frac{\Delta p}{\tau_p} + G_L$$

Minority Carrier Diffusion Equation

The minority carrier diffusion equations are derived from the general continuity equations, and are applicable only for minority carriers.

Simplifying assumptions

1. The electric field is small, such that

$$J_N = q\mu_n n\mathcal{E} + qD_N\frac{\partial n}{\partial x} \cong qD_N\frac{\partial n}{\partial x} \qquad \text{in p-type material}$$

$$J_P = q\mu_p p\mathcal{E} + qD_P\frac{\partial p}{\partial x} \cong qD_P\frac{\partial p}{\partial x} \qquad \text{in n-type material}$$

2. n_0 and p_0 are independent of x (uniform doping)
3. low-level injection conditions prevail

Starting with the continuity equation for electrons

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_N(x)}{\partial x} - \frac{\Delta n}{\tau_n} + G_L \rightarrow \frac{\partial(n_0+\Delta n)}{\partial t} = \frac{1}{q}\frac{\partial}{\partial x}\left[qD_N\frac{\partial(n_0+\Delta n)}{\partial x}\right] - \frac{\Delta n}{\tau_n} + G_L$$

$$\frac{\partial \Delta n}{\partial t} = D_N\frac{\partial^2 \Delta n}{\partial x^2} - \frac{\Delta n}{\tau_n} + G_L$$

Minority Carrier Diffusion Equation

The subscript “n” or “p” is used to explicitly denote n-type or p-type material, e.g.

p_n is the hole (minority-carrier) concentration in n-type material

n_p is the electron (minority-carrier) concentration in p-type material

Thus the minority carrier diffusion equations are

$$\frac{\partial \Delta n_p}{\partial t} = D_N \frac{\partial^2 \Delta n_p}{\partial x^2} - \frac{\Delta n_p}{\tau_n} + G_L \qquad \text{in p-type material}$$

$$\frac{\partial \Delta p_n}{\partial t} = D_P \frac{\partial^2 \Delta p_n}{\partial x^2} - \frac{\Delta p_n}{\tau_p} + G_L \qquad \text{in n-type material}$$

Simplifications (Special Cases):

Steady state:

$$\frac{\partial \Delta n_p}{\partial t} = 0 \ , \ \frac{\partial \Delta p_n}{\partial t} = 0$$

No diffusion current:

$$D_N \frac{\partial^2 \Delta n_p}{\partial x^2} = 0 \ , \ D_P \frac{\partial^2 \Delta p_n}{\partial x^2} = 0$$

No R-G:

$$\frac{\Delta n_p}{\tau_n} = 0 \ , \frac{\Delta p_n}{\tau_p} = 0$$

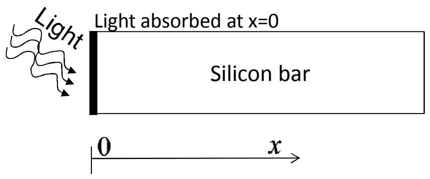
No light:

$$G_L = 0$$

Example

Consider the special case:

1. constant minority-carrier (hole) injection at x=0
2. steady state; no light absorption for x>0 $\Delta p_n(0) = \Delta p_{n0}$



$$0 = D_P \frac{\partial^2 \Delta p_n}{\partial x^2} - \frac{\Delta p_n}{\tau_p}$$

$$\frac{\partial^2 \Delta p_n}{\partial x^2} = \frac{\Delta p_n}{D_P \tau_p} = \frac{\Delta p_n}{L_P{}^2}$$

L_P is the ***hole diffusion length***: $L_P \equiv \sqrt{D_P \tau_p}$

The general solution to the equation is

$$\Delta p_n(x) = A e^{-x/L_P} + B e^{x/L_P}$$

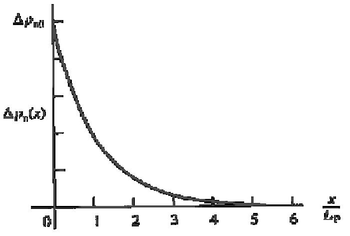
where A, B are constants determined by boundary conditions:

BC: $\Delta p_n(\infty) = 0 \quad \Rightarrow \quad B = 0$

$\Delta p_n(0) = \Delta p_{n0} \quad \Rightarrow \quad A = \Delta p_{n0}$

Hence solution is:

$$\Delta p_n(x) = \Delta p_{n0} A e^{-x/L_P}$$



Example - Minority Carrier Diffusion Length

Physically, L_P and L_N represent the average distance that minority carriers can diffuse into a sea of majority carriers before being annihilated.

Q: Find L_P if N_D=10^{16} cm^{-3}; t_p = 10^{-6} s

$$L_P \equiv \sqrt{D_P \tau_p}$$

$$D_P = \frac{kT}{q}\mu_p$$

$$\mu_p = 400\,cm^2/Vs$$

$$D_p = 10\,cm^2/s$$

$$L_p = 30\,\mu m$$

Quasi-Fermi Levels

Whenever Dn = Dp ≠ 0, $np \neq n_i^2$. However, we would like to preserve and use the relations:

$$n = n_i e^{(E_F - E_i)/kT} \qquad p = n_i e^{(E_i - E_F)/kT}$$

These equations imply $np = n_i^2$, however. The solution is to introduce two ***quasi-Fermi levels*** F_N and F_P such that

$$n = n_i e^{(F_N - E_i)/kT} \qquad p = n_i e^{(E_i - F_P)/kT}$$

$$F_N \equiv E_i + kT\ln\left(\frac{n}{n_i}\right) \qquad F_P \equiv E_i - kT\ln\left(\frac{p}{n_i}\right)$$

Example: Quasi-Fermi Levels

Consider a Si sample with N_D = 10^{17} cm^{-3} and D*n* = D*p* = 10^{14} cm^{-3}.

What are p and n ?

$$n_0 = N_D = 10^{17}\,cm^{-3},\, p_0 = n_i^2 / n_0 = 10^3\,cm^{-3}$$
$$n = n_0 + \Delta n = 10^{17} + 10^{14} \approx 10^{17}\,cm^{-3}$$
$$p = p_0 + \Delta p = 10^3 + 10^{14} \approx 10^{14}\,cm^{-3}$$

What is the np product ?

$$np = 10^{31}\,cm^{-3}$$

Find F_N and F_P :

$$F_N \equiv E_i + kT \ln\left(n/n_i\right) \rightarrow F_N - E_i = kT \ln\left(10^7\right) = 0.42eV$$
$$F_P \equiv E_i - kT \ln\left(p/n_i\right) \rightarrow E_i - F_P = kT \ln\left(10^4\right) = 0.24eV$$