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Karlsruhe Institute of Technology

Optical Transmitters and Receivers (OTR)
Tutorial on Semiconductor Basics

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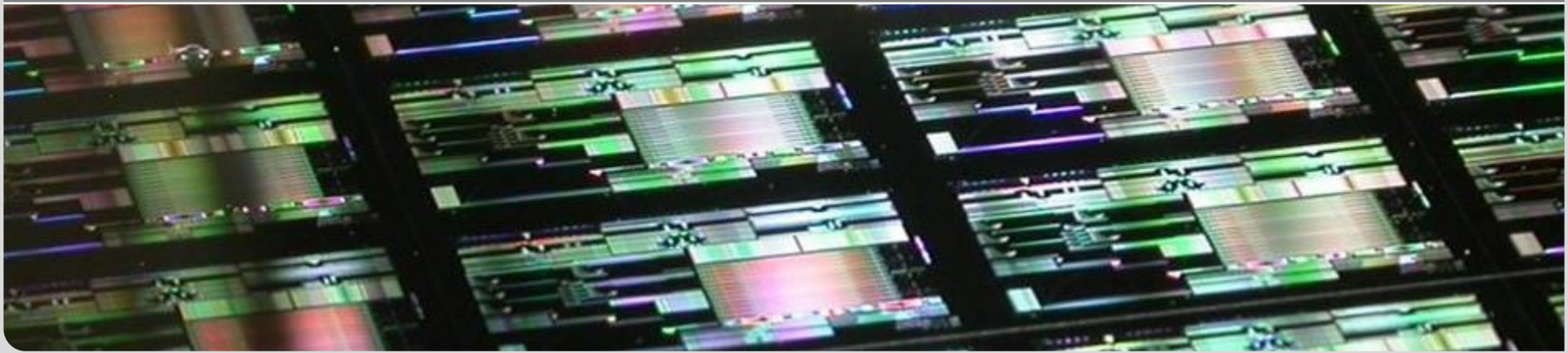
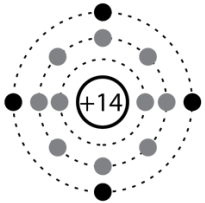


Content

- Band Diagrams, Band structure
- Density of states
  - Effective density of states
- Fermi-Dirac Distribution
  - Boltzmann approximation
- Doping, pn-junction formation and current-voltage characteristics

Silicon atom energy levels

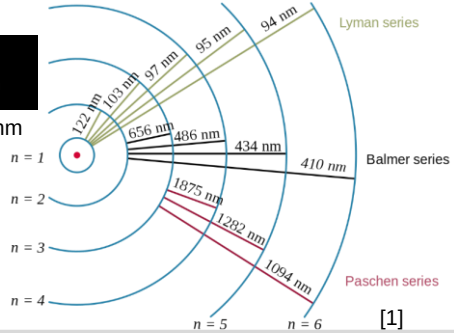
- Si atom :
  - 14 positive charges in the nucleus
  - 14 electrons residing in shells around the nucleus (principal quantum numbers n = 1, 2, 3, and 4)



Shells $n = 1,2, \ldots$
Maximum number of electrons: $2n^2$
But maximum 8 in the most outer shell

Balmer series of hydrogen atom:

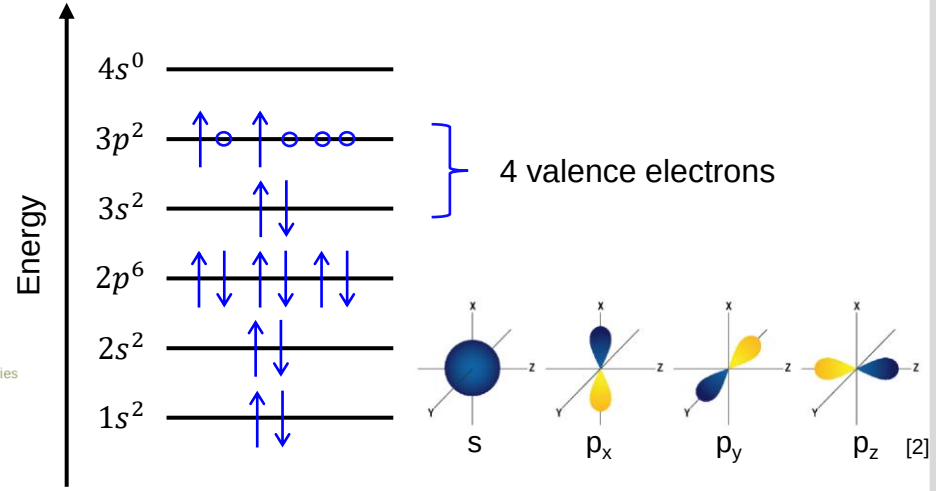
410 nm 434 nm 486 nm 656 nm



[1]

$$W = hf = h\frac{c}{\lambda} \rightarrow \lambda = h\frac{c}{W}$$

- Each orbital possesses a distinct energy level



[2]

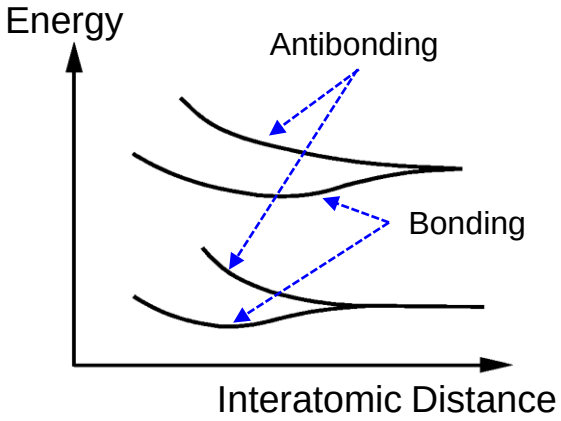
Subshells $l = 0,1,2, \ldots (s, p, d \ldots)$
Maximum 2 electrons in each orbital

[1] Wikipedia
[2] Wijeratne, K. (2018). Conducting Polymer Electrodes for Thermogalvanic Cells (PhD dissertation, Linköping University Electronic Press). https://doi.org/10.3384/diss.diva-152888

Atoms forming bonds

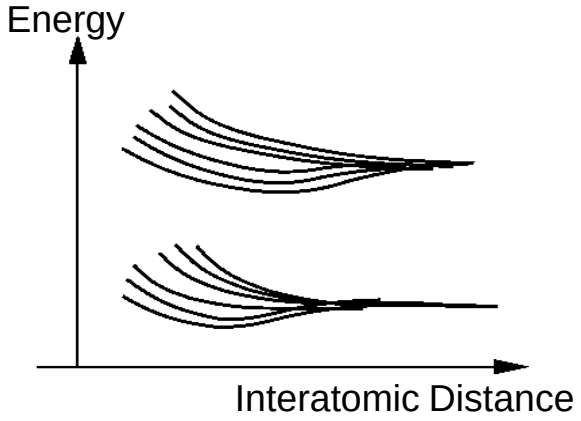
When atoms come closer to each other to form bonds: Atomic orbital energy levels split into bonding and antibonding orbitals (Pauli's exclusion principle)

For 2 atoms:



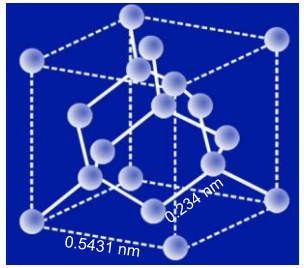
For 6 atoms:

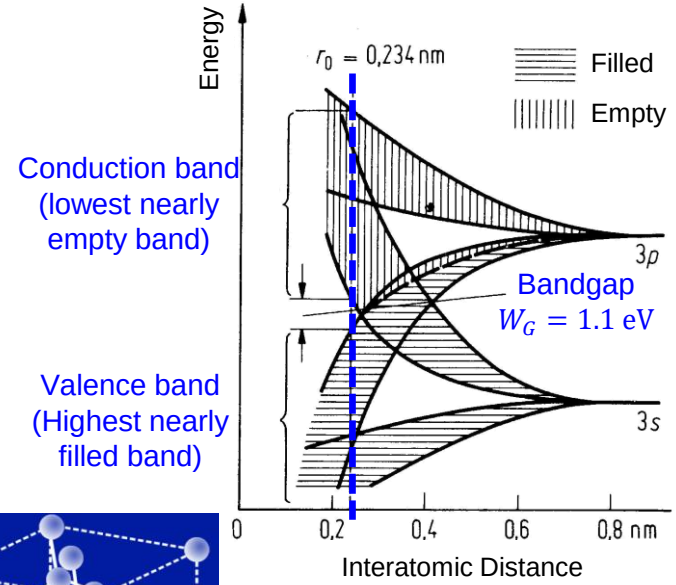
Splitting into 6 discrete energy levels



Pure Si crystal
energy levels ⟹ energy bands

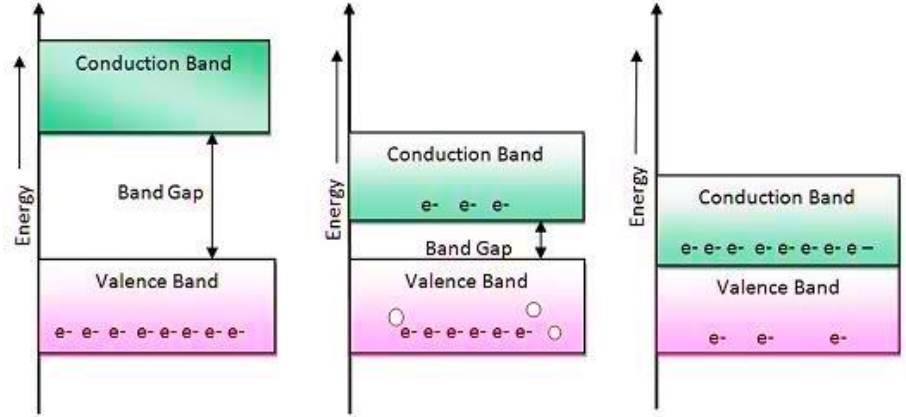
- When silicon atoms are put together in a lattice, the orbitals of adjacent atoms interact.
- Atom density of silicon is $5 \times 10^{22} \mathrm{cm}^{-3}$.
- The 3s- and 3p-states split into 5×10^{22} different energy levels.
- Half of these states move lower in energy and form bonding states. They are occupied by electrons.
- An equal number of unoccupied states are higher up in energy.
- At the minimum atomic distance of the Si crystal (d = 0.234 nm at T = 0 K, lattice constant a = 0.54 nm) a band gap W_G =1.1 eV void of energy levels is formed.
- Discrete, but densely spaced energy states of a Si atom are represented by energy bands above (conduction band) and below the bandgap (valence band).





Insulators, semiconductor and metals

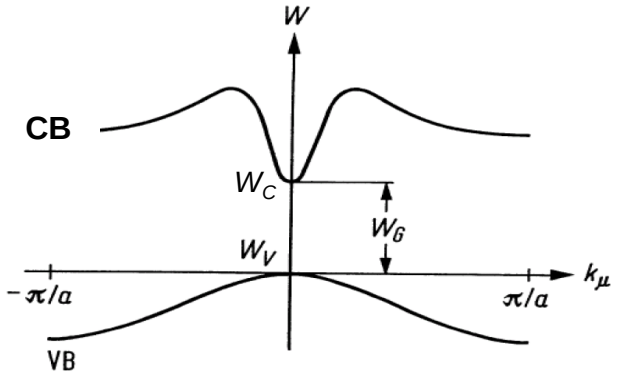
- **Insulator:** Large bandgap, (almost) no electron states occupied in conduction band, fully occupied electron states in valence band
- **Semiconductor:** Smaller bandgap, valence band and conduction band partially filled due to thermal excitation at room temperature T = 293 K
- **Metal:** At T = 0 K conduction band partially occupied, or even overlapping with valence band



Insulator Semiconductor Metal

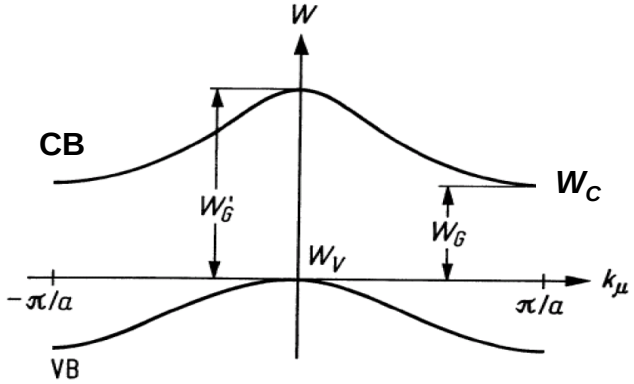
Direct and indirect semiconductors

Direct semiconductor (e.g. GaAs, InP)



- Quantity k_μ is the propagation constant of the electronic wave inside the crystal. Linear electron momentum in crystal is $\hbar k_\mu$ (de Broglie)
- Maximum of valence band and minimum of conduction band at same momentum $\hbar k_\mu$.
- Very probable transition, energy and crystal momentum conserved. If transition is radiative, then material is usable for light emission.

Indirect semiconductor (e.g. Si, Ge)



- Maximum of valence band and minimum of conduction band at different momentum $\hbar k_\mu$.
- For a transmission from $W_{C,min} \rightarrow W_{V,max}$, a momentum change of $\hbar\pi/a$ is required.
- Momentum of a photon: $\hbar 2\pi/\lambda$, with $\lambda >> a$
- Third particle needed (phonon) for crystal momentum conservation, unlikely transition

Density of states

Density of states: Number of available energy states per energy interval and volume

ρ_C: density of energy states per energy interval in conduction band

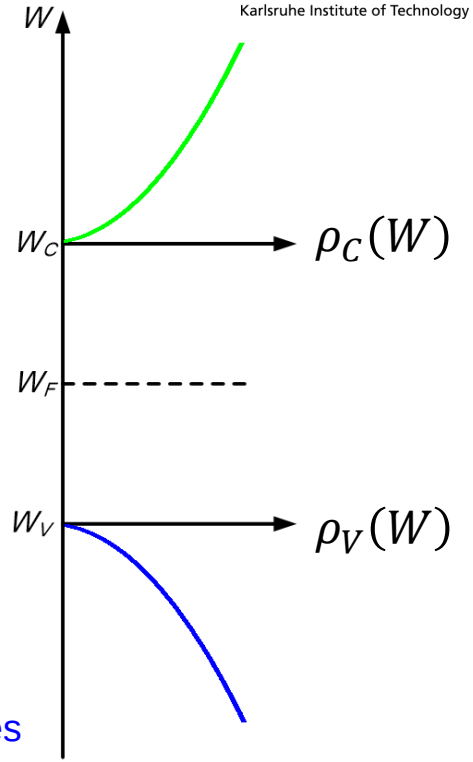
ρ_V: density of energy states per energy interval in valence band

$$\rho_C(W) = \frac{1}{2\pi^2}\left(\frac{2m_n}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{W - W_C}$$

$$\rho_V(W) = \frac{1}{2\pi^2}\left(\frac{2m_p}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{W_V - W}$$

$m_{n,p}$: effective mass of electron (hole) moving through periodic crystal potential

Density of states increases with increasing energetic distance from band edges



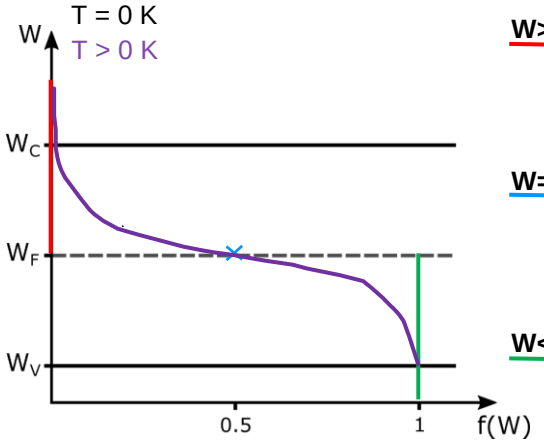
Fermi-Dirac distribution

The occupation probability of electrons in available energy states in a band is given by the Fermi-Dirac distribution

$$f(W) = \frac{1}{1 + e^{\frac{W - W_F}{kT}}}$$

k	Boltzmann's constant
kT	Thermal energy, 25 meV at $T = 293$ K
W_F	Fermi energy

- $f(W)$ describes the probability that a state at energy W is occupied by an electron.
- W_F is called the **Fermi energy** where the occupation probability is $1/2$ at all temperatures.
- In equilibrium, the Fermi energy is a material constant. It changes if we move from intrinsic to doped semiconductors

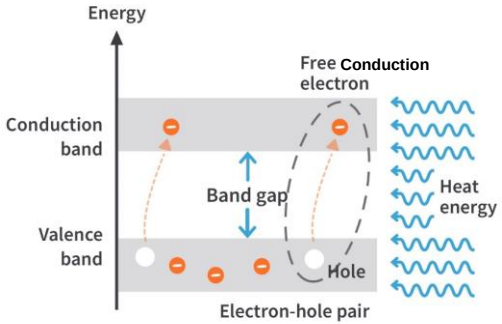


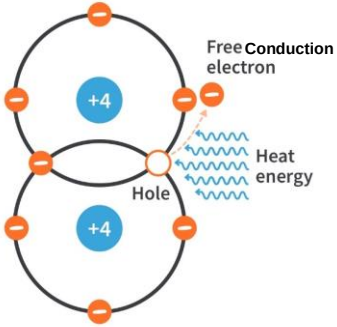
W>W$_F$: $\lim_{T\to 0} f(W) = \frac{1}{1 + e^{\frac{W - W_F}{kT}}} = 0$ ($e^{\frac{W-W_F}{kT}} \to \infty$)

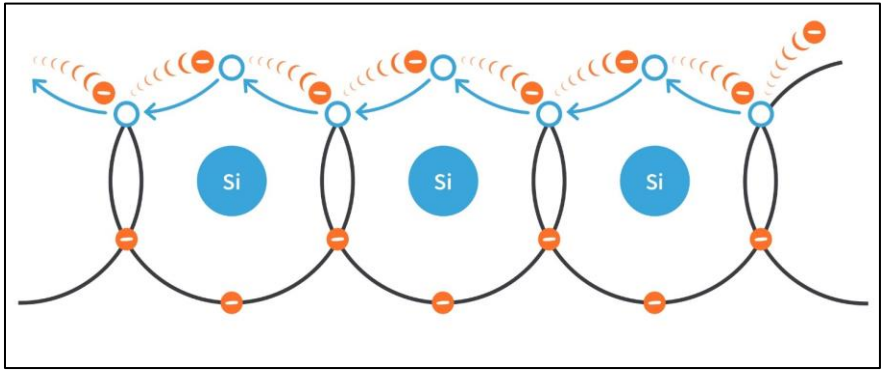
W=W$_F$: $\lim_{T\to 0} f(W) = \frac{1}{1 + e^{\frac{0}{kT}}} = \frac{1}{2}$ ($e^{\frac{0}{kT}} \to 1$)

W<W$_F$: $\lim_{T\to 0} f(W) = \frac{1}{1 + e^{\frac{W - W_F}{kT}}} = 1$ ($e^{\frac{W-W_F}{kT}} \to 0$)

Creation of electron-hole pair







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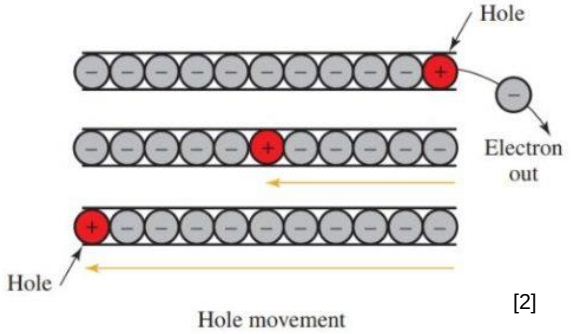
Electron and holes are generated at the same spatial position in crystal

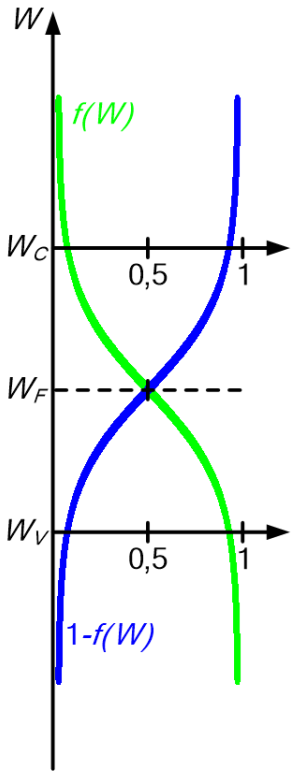


[2]

[1] Introduction to Electronics - Study Guides | CircuitBread
[2] Semiconductor Basics Tutorial | Electrical Academia

Fermi-Dirac distribution: intrinsic semiconductor

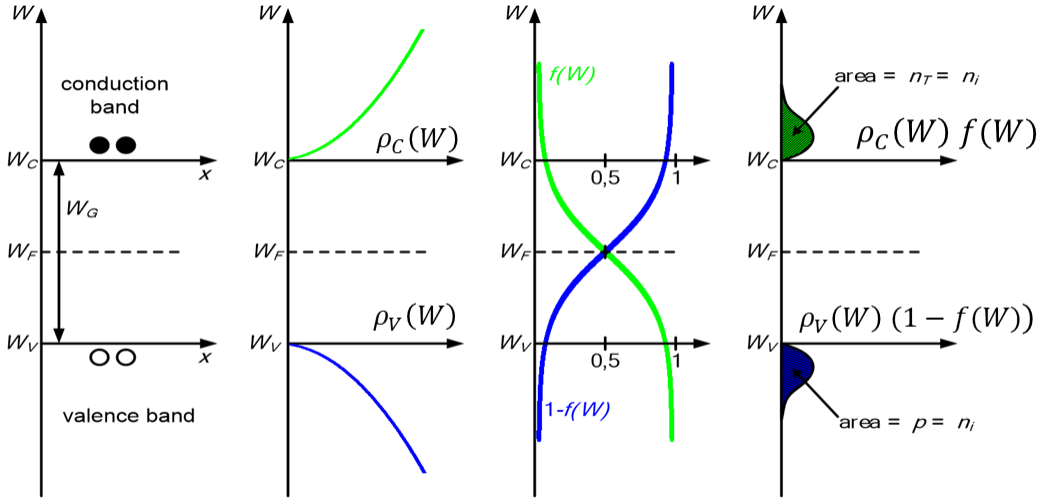
- Intrinsic semiconductor - Fermi level located in the middle of the bandgap
- Symmetry of the probability distribution → probability of finding an electron in CB equal to probability of finding a hole in VB
- $f_V(W) = 1 - f(W)$ is the probability that a state at energy W is **not occupied** by an electron (empty state)
- As an empty energy state in the valence band is called a “hole”, $f_V(W)$ gives the probability of finding a hole in the valence band



Carrier concentration (intrinsic semiconductor)

- In semiconductors, both the electrons in the CB and the holes in the VB contribute to conduction.
- *Carrier concentration* in conduction band (n_T) and valence band (p):

$$n_T = \int_{W_C}^{\infty} \rho_C(W)\, f(W)\, \mathrm{d}W \qquad p = \int_{-\infty}^{W_V} \rho_V(W)\, [1 - f(W)]\, \mathrm{d}W$$



Effective density of states

Simplification of the density of states function

- Assuming all the states are located near the band edge W_c and W_V
- Result: Effective density of states in conduction band (N_c) and in valence band (N_V).

$$N_C = 2\left(\frac{2\pi m_n kT}{h^2}\right)^{3/2}$$

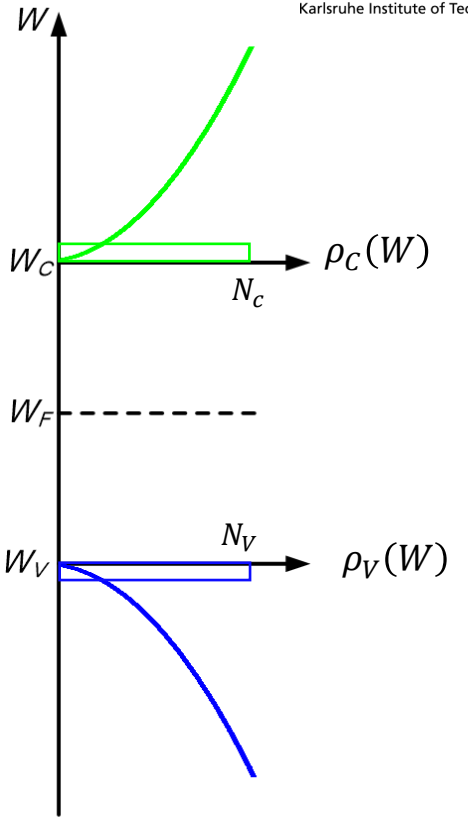
$$N_V = 2\left(\frac{2\pi m_p kT}{h^2}\right)^{3/2}$$

Only T is variable

$m_{n,p}$: Effective mass of electron and hole

h : Planck's constant

k : Boltzmann constant



Typical values for GaAs at T = 293 K

$N_c \approx 10^{17}$ cm^{-3}

$N_V \approx 10^{18}$ cm^{-3}

Boltzmann approximation

Simplification of the Fermi-Dirac distribution

$$f(W) = \frac{1}{1 + \mathrm{e}^{\frac{W - W_F}{kT}}}$$

- kT is usually a small number ≈ 25 meV at 293K
- As long as $W - W_F \gg kT$ the exponential term in the denominator dominates
- If Fermi level is far away ($> 3kT$) from the band edges W_C and W_V **Boltzmann's approximation holds**:

$$\frac{1}{1 + \mathrm{e}^{x}} \underset{x \gg 1}{\approx} \frac{1}{\mathrm{e}^{x}} \quad \Rightarrow \quad f_{C,e}(W) \approx \mathrm{e}^{-\frac{W - W_F}{kT}}$$

$$f_{V,p}(W) \approx \mathrm{e}^{-\frac{W_F - W}{kT}}$$

- **Note:** $f_{V,p}(W) = 1 - f(W)$ is not valid when Boltzmann's approximation is used
- Carrier concentration:

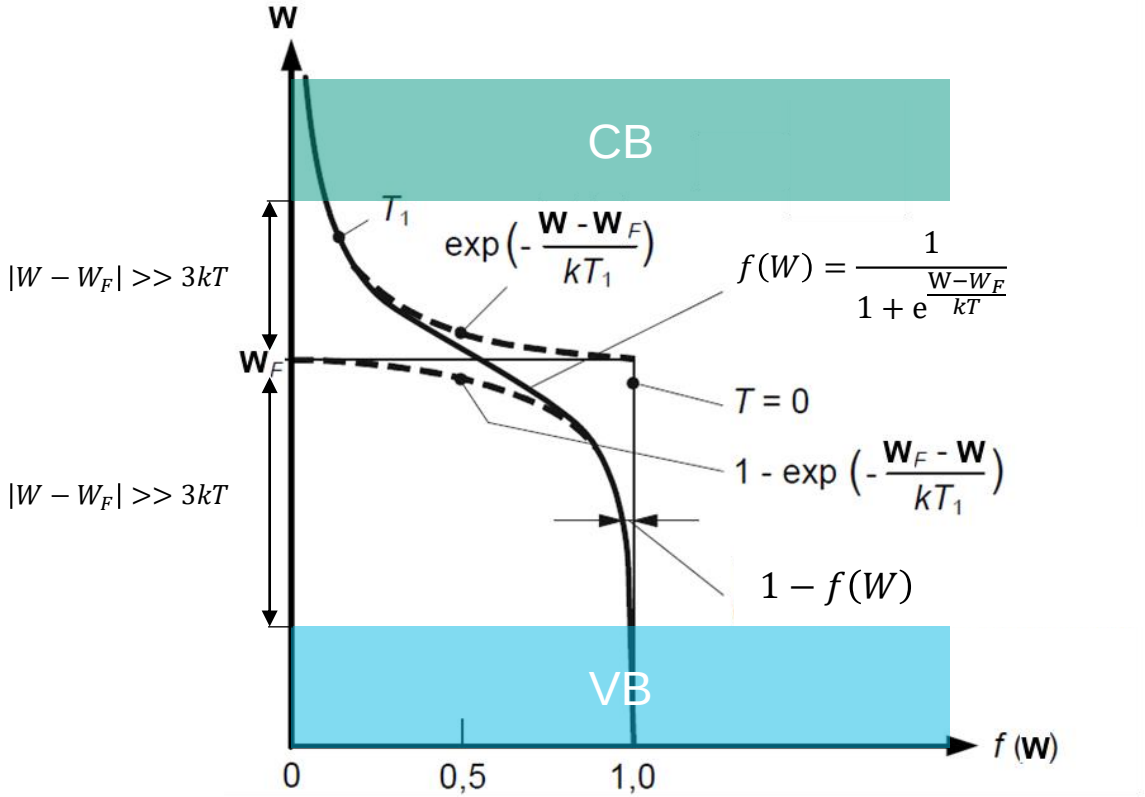
$$n_T \approx N_C \mathrm{e}^{-\frac{W_C - W_F}{kT}}$$

$$p \approx N_V \, \mathrm{e}^{-\frac{W_F - W_V}{kT}}$$

$$n_T = p = n_i = \sqrt{n_T p} = \sqrt{N_C N_V}\, e^{-\frac{W_G}{2kT}}$$

n_i increases with increasing T
n_i decreases with increasing W_G

Boltzmann approximation graphical representation



Doping

- Intrinsic semiconductor: Pure semiconductor with negligible amount of impurities. Electron and hole carrier concentrations in thermal equilibrium are determined by material properties and temperature.

$$n_T = p = n_i = \sqrt{n_T p} = \sqrt{N_C N_V}\, e^{-\frac{W_G}{2kT}}$$

$W_G\ (\mathrm{Si}) = 1.1\ \mathrm{eV}$

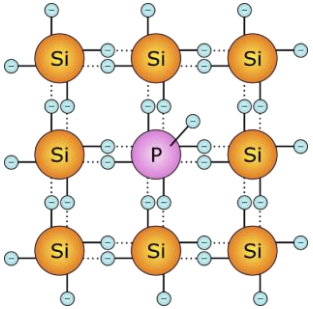
$W_G\ (\mathrm{GaAs}) = 1.4\ \mathrm{eV}$

$n_i\ (\mathrm{Si}) = 1 \times 10^{10}\mathrm{cm}^{-3}$; T = 300K

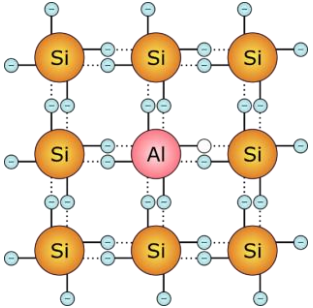
$n_i\ (\mathrm{GaAs}) = 2 \times 10^{6}\mathrm{cm}^{-3}$; T = 300K

- Extrinsic semiconductor: Doping changes carrier concentrations in thermal equilibrium. *Donors* "donate" negatively charged electrons to the conduction band (n-type). *Acceptors* "accept" additional electrons and positively charged "holes" are created in the valence band (p-type).

n-type



p-type



Doping

- *Neutrality* condition: the density of negative particles and positive particles should be equal. there are four types of charged species in a doped semiconductor: electrons, holes, donor ions, acceptor ions.

$$n_T + n_A^- = p + n_D^+$$

ionized acceptor atoms: additional holes

ionized donor atoms: additional electrons

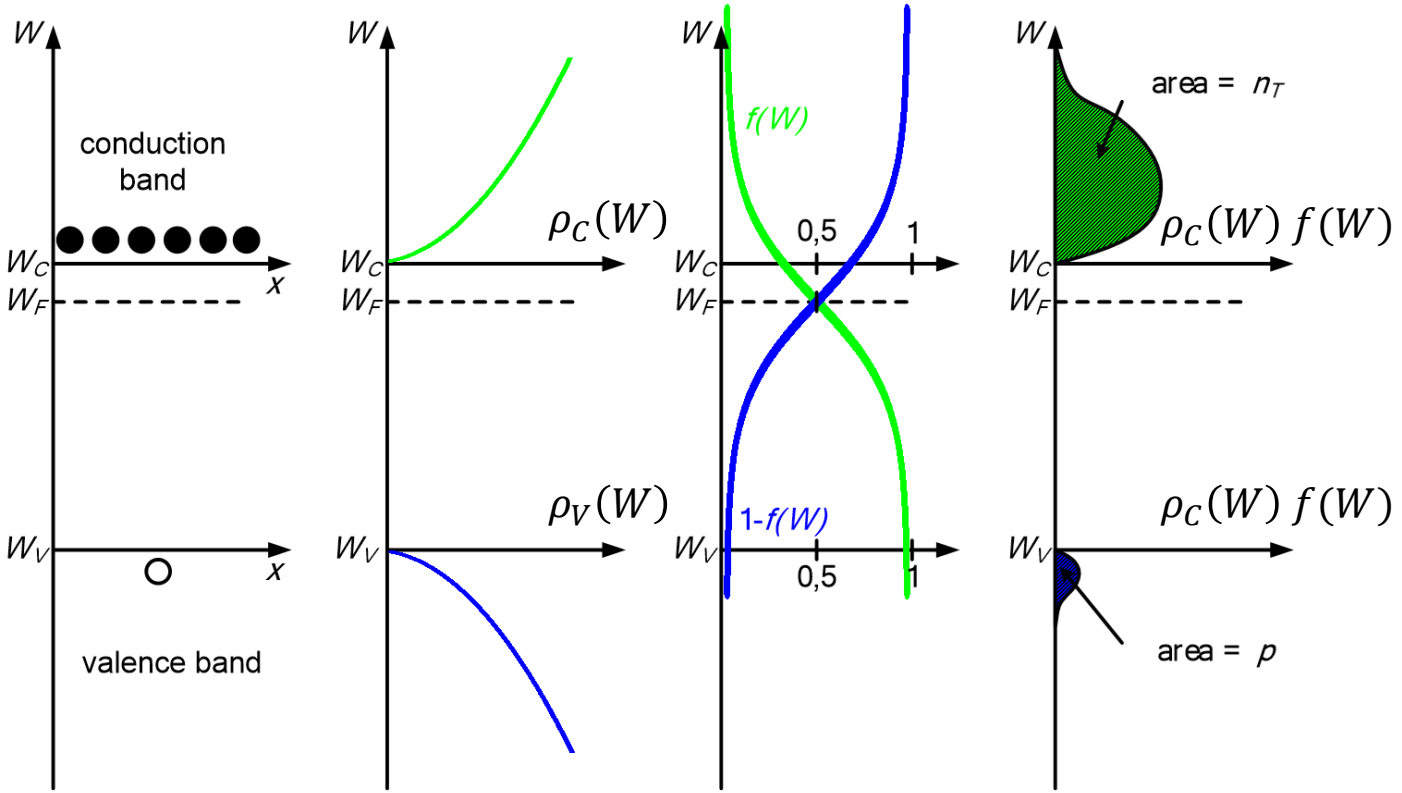
- *Mass-action law* holds in thermal equilibrium for intrinsic *and* (non-degenerately doped) extrinsic semiconductors:

$$n_T p = n_i^2$$

- At room temperature:

n-type:	$n_D^+ - n_A^- \gg n_i$	p-type:	$n_A^- - n_D^+ \gg n_i$
majorities:	$n_T \approx n_D$	majorities:	$p \approx n_A$
minorities:	$p_{n0} \approx n_i^2/n_D$	minorities:	$n_{p0} \approx n_i^2/n_A$

n-type semiconductor in thermal equilibrium



Currents in semiconductors

- Drift current density due to an electric field $\vec{E}$ acting on the carriers

$$\vec{J}_F = \vec{J}_{n,F} + \vec{J}_{p,F} = \underbrace{(en_T\mu_n + ep\mu_p)}_{=:\sigma}\vec{E}$$

$\mu_{n,p}$	carrier mobility
e	elementary charge
σ	conductivity

- Diffusion current density due to a gradient in carrier concentration

$$\vec{J}_D = \vec{J}_{n,D} + \vec{J}_{p,D} = eD_n \,\mathrm{grad}\, n_T - eD_p \,\mathrm{grad}\, p$$

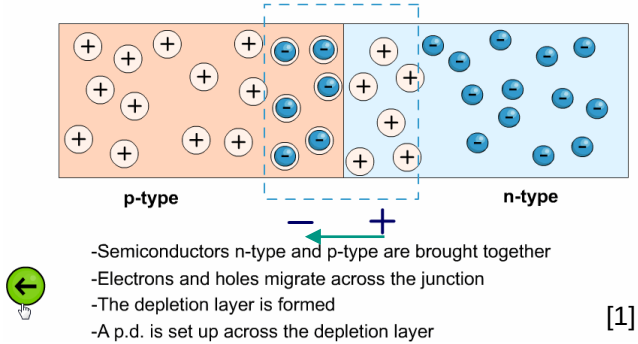
Diffusion coefficients

$$D_{n,p} = \mu_{n,p} U_T = \mu_{n,p} \frac{kT}{e}, where\ kT = 25\ mV$$

pn-Junction in thermal equilibrium

- Electrons diffuse into the p-type semiconductor, and holes into the n-type semiconductor.
- The positively and negatively charged donor and acceptor ions in the space charge region (SCR) build up an electric field that counteracts diffusion.
- In thermal equilibrium, there are zero net electron and hole currents, i.e., diffusion and drift currents compensate each other:

$$\vec{J}_{n,F} + \vec{J}_{n,D} = \vec{0}, \qquad \vec{J}_{p,F} + \vec{J}_{p,D} = \vec{0}$$



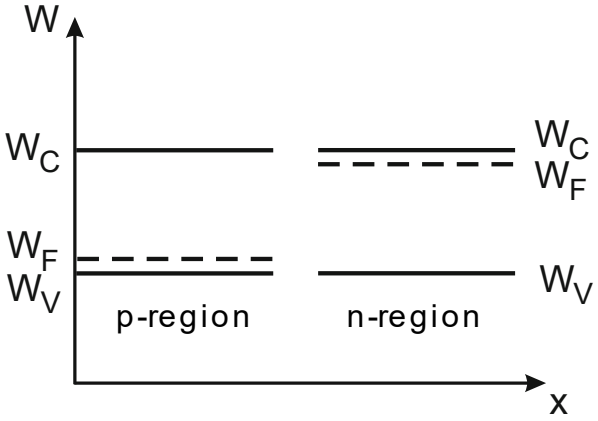
[1]

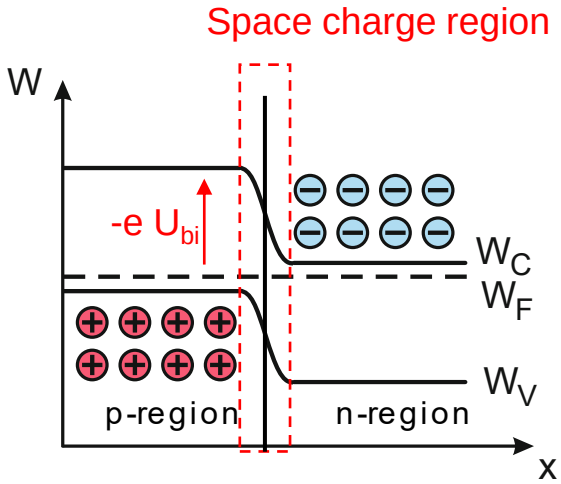
[1] *A. Ahmed, "Forming a P-N Junction of Diode !," IAMTECHNICAL. http://iamtechnical.com/forming-p-n-junction-diode (accessed May 28, 2020).*

pn-Junction in thermal equilibrium

Thermal equilibrium ($U = 0$)

- p and n-type are brought in contact
- Space charge region is formed
- Built-in potential is created
- Fermi level is aligned





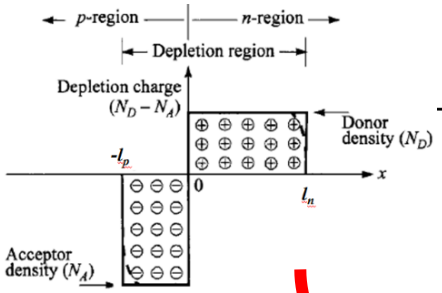
Diffusion and drift currents compensate each other

U_{bi} : Built-in potential

Adapted from H. Göbel, Einführung in die Halbleiter-Schaltungstechnik. Berlin, Heidelberg: Springer Berlin Heidelberg, 2019.

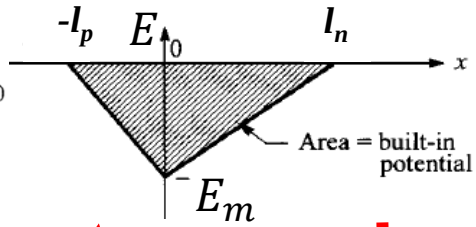
pn-Junction in thermal equilibrium

Charge density ρ



Electric field E

$$\varepsilon E = \int \rho \, \mathrm{d}x$$

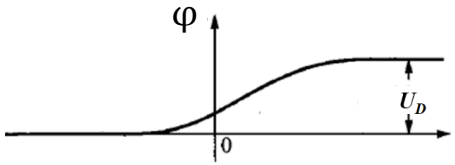


Integration

Potential

$$\vec{E} = -\mathrm{grad}\varphi = -\frac{\mathrm{d}\varphi}{\mathrm{d}x}$$

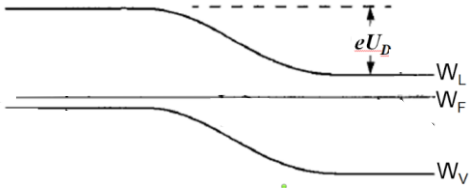
$$\varphi = -\int E \, \mathrm{d}x$$



Integration

Energy diagram

$$W_C(x) = W_C - e\varphi(x)$$

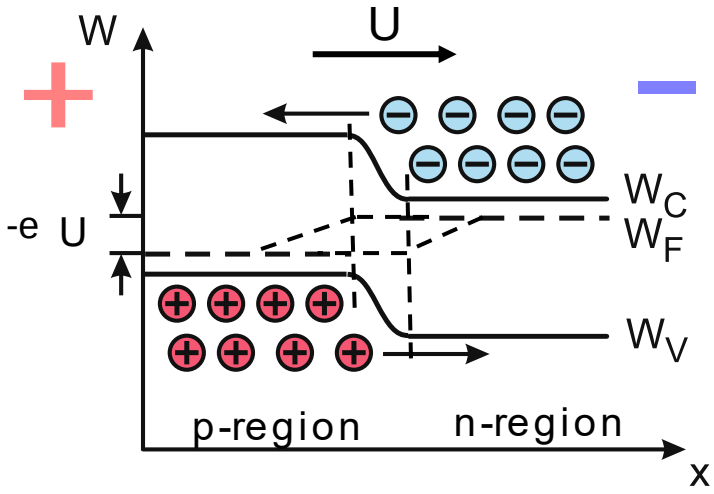


The *built-in potential* U_{bi} of the pn-junction is given by:

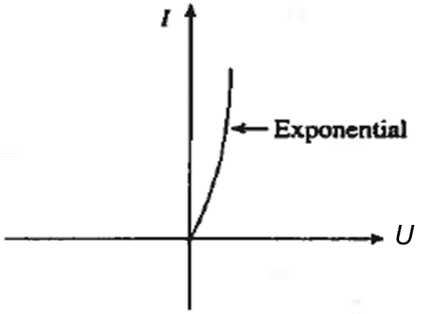
$$U_{bi} = U_T \ln \frac{n_D n_A}{n_i^2} = \frac{kT}{e} \ln \frac{n_D n_A}{n_i^2}$$

pn-Junction in forward bias

Forward bias ($U > 0$)



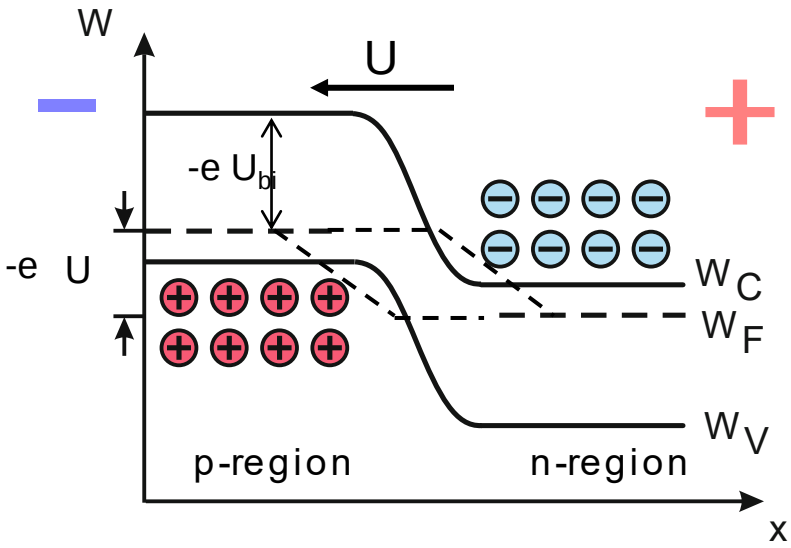
- Fermi level split into quasi fermi levels
- Potential becomes smaller for U > 0
  → increased diffusion current
- Strong gradient of carriers
- Diffusion current dominates



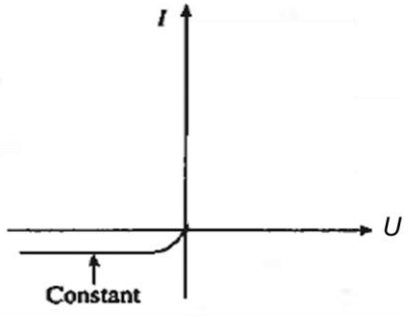
Adapted from H. Göbel, Einführung in die Halbleiter-Schaltungstechnik. Berlin, Heidelberg: Springer Berlin Heidelberg, 2019.

pn-Junction in reverse bias

Reverse bias ($U < 0$)



- Potential becomes larger for U < 0
  → Energy difference of -e ($U+U_{bi}$)
  → reduced diffusion current

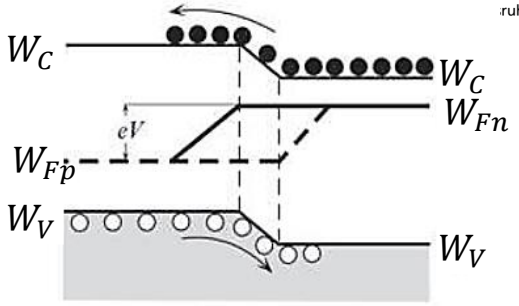


Adapted from H. Göbel, Einführung in die Halbleiter-Schaltungstechnik. Berlin, Heidelberg: Springer Berlin Heidelberg, 2019.

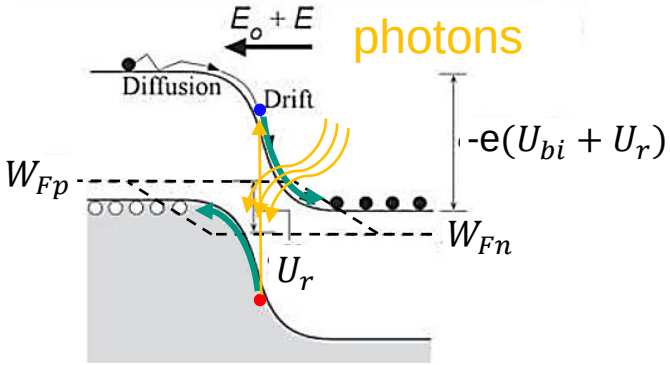
pn-Junction: quasi Fermi levels

- If external voltage is applied, the Fermi level is no longer constant over the whole semiconductor
- Inside the space charge region, quasi Fermi levels occur, which describe hole and electron concentrations in valence and conduction band independently
- Forward bias: Within the space charge region it is now possible to have a high number of electrons and holes at the same time
- Reverse bias: within the space charge region, the carriers are separated before they have the chance to recombine

Forward Bias:

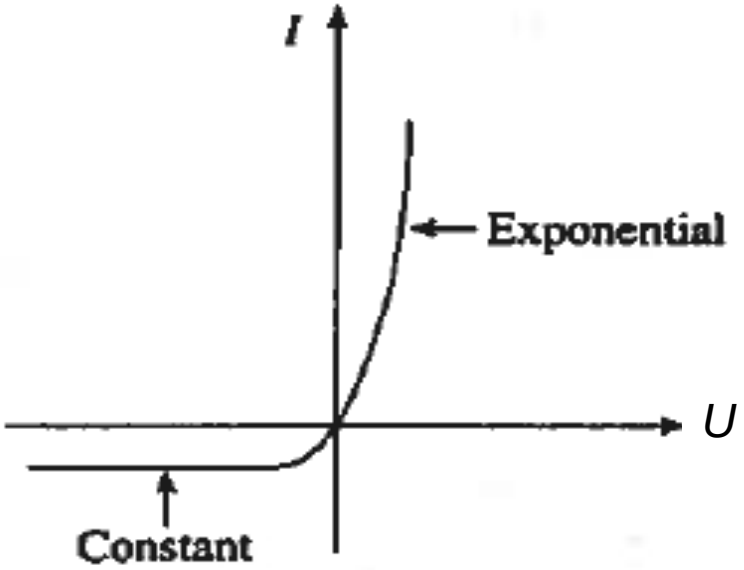


Reversed Bias:



Adapted from Optoelectronics and Photonics: Principles and Practices by S.O. Kasap, 2nd Ed. (Fig. 3.26)

pn-Junction



$$I = I_S\left(\exp\left(\frac{eU}{kT}\right) - 1\right)$$

I_s Reverse saturation current