Lecture contents

- Semiconductor statistics
- Transport

Statistics of carriers: General

Electron concentration at the energy E
(Density of states) x (distribution function):

$$n(E) = N_c(E) f(E)$$

Electron concentration in the energy range E to $E+dE$ close to the conduction band minimum:

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

Total electron concentration in the conduction band

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

$$x = \frac{E - E_C}{k_B T} \qquad \eta_c = \frac{E_F - E_C}{k_B T}$$

$$= \frac{\sqrt{2} m_e^{*3/2}}{\pi^2 \hbar^3} (k_B T)^{3/2} \int_0^{\infty} \frac{x^{1/2} dx}{\exp(x - \eta_c) + 1} =$$

$$= 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2} \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{x^{1/2} dx}{\exp(x - \eta_c) + 1}$$

General equation for carrier concentration
(effective density of states) x (Fermi integral of ½ order):

$$n = N_C \Phi_{1/2}(\eta_c)$$

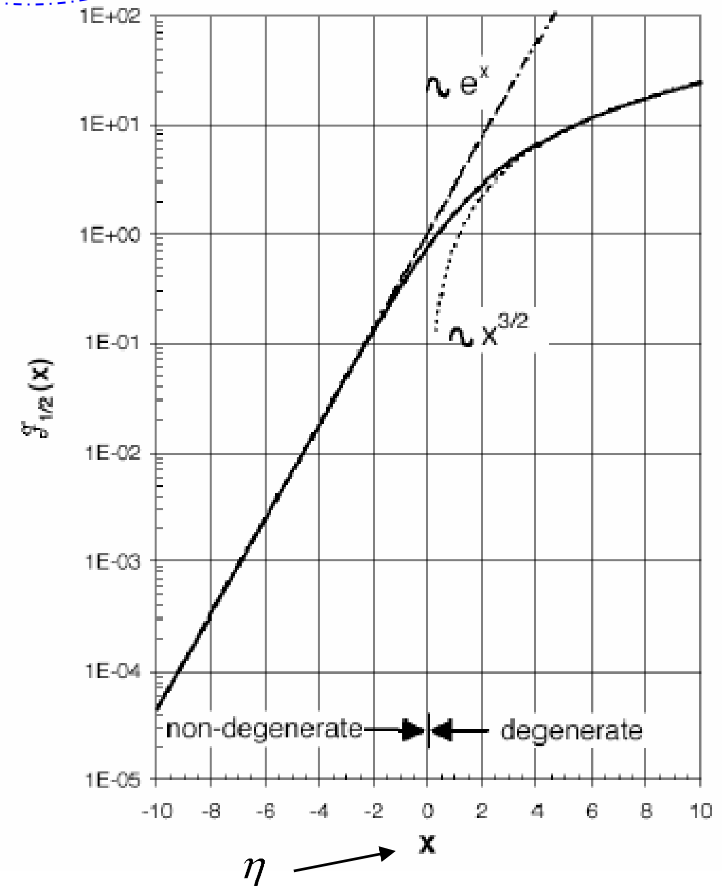
Statistics of carriers: General

The same is true for holes in the valence band:

$$p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}dx}{\exp(x-\eta_V)+1}$$

$$p = N_V \Phi_{1/2}(\eta_V)$$

$\Phi_{1/2}(\eta)$

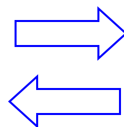


Effective density of states of electrons (or holes)

$$N_c = 2.512 \times 10^{19} \left(\frac{m_{dn}}{m_e}\right)^{3/2} \left(\frac{T}{300}\right)^{3/2} \left(cm^{-3}\right)$$

One-to-one correspondence

Concentration of mobile (band) carriers



Fermi level position

Statistics of carriers: Non-degenerate system

General equation:

$$n = N_C \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2} dx}{\exp(x - \eta_c) + 1} \qquad x = \frac{E - E_C}{k_B T} \qquad \eta_c = \frac{E_F - E_C}{k_B T}$$

If all the C.B. energies are far from Fermi level:
$E_C - E_F >> k_B T \quad (> 3\, k_B T)$:

$$\exp(x - \eta_c) >> 1$$

$$\int_0^\infty \frac{x^{1/2} dx}{\exp(x - \eta_c) + 1} = \int_0^\infty e^{-(x-\eta_c)} x^{1/2} dx = e^{\eta_c} \int_0^\infty e^{-x} x^{1/2} dx = e^{\eta_c} \frac{\sqrt{\pi}}{2}$$

<u>Concentration of band carriers</u>

General case:

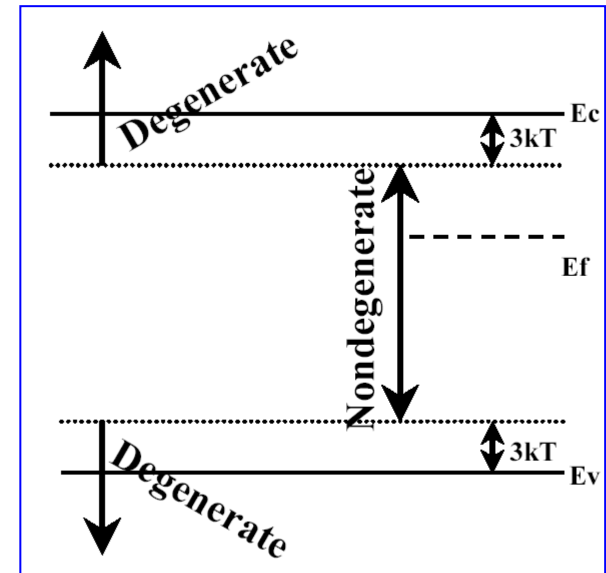
$$n = N_C \Phi_{1/2}(\eta_c)$$

$$p = N_V \Phi_{1/2}(\eta_V)$$

Non-generate system:

$$n = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right)$$

$$p = N_V \exp\left(\frac{E_V - E_F}{k_B T}\right)$$

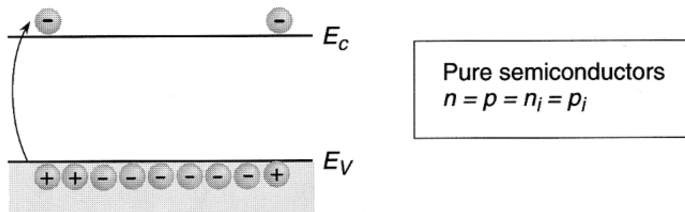


$$np = N_C N_V \exp\left(-\frac{E_g}{k_B T}\right) \equiv n_i^2$$

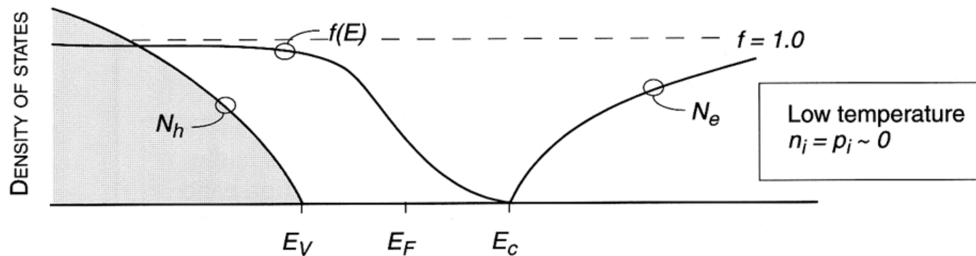
Definition of intrinsic carrier concentration

Carriers in intrinsic semiconductors

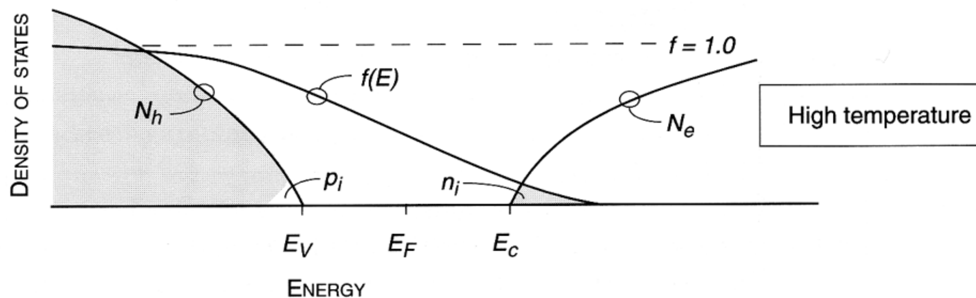
Material	Conduction band effective density (N_C)	Valence band effective density (N_V)	Intrinsic carrier concentration ($n_i = p_i$)
Si (300 K)	2.78 x 10^{19} cm^{-3}	9.84 x 10^{18} cm^{-3}	1.5 x 10^{10} cm^{-3}
Ge (300 K)	1.04 x 10^{19} cm^{-3}	6.0 x 10^{18} cm^{-3}	2.33 x 10^{13} cm^{-3}
GaAs (300 K)	4.45 x 10^{17} cm^{-3}	7.72 x 10^{18} cm^{-3}	1.84 x 10^{6} cm^{-3}



Pure semiconductors
$n = p = n_i = p_i$

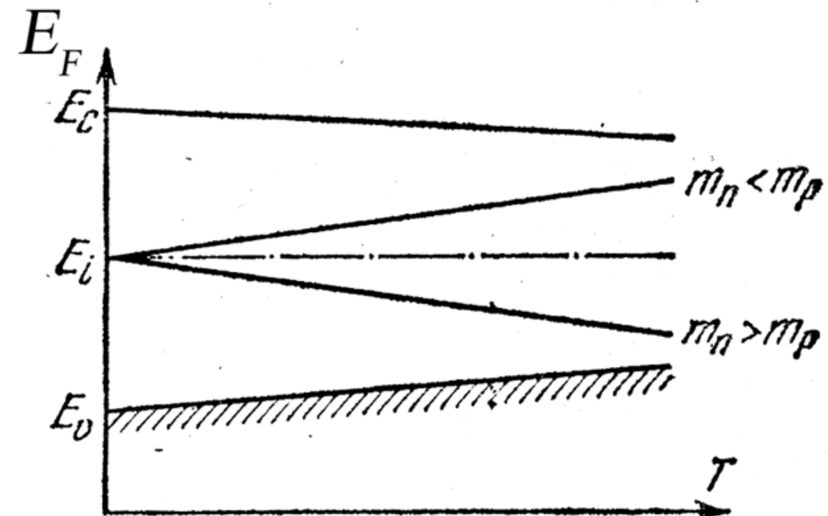


Low temperature
$n_i = p_i \sim 0$



High temperature

Fermi level position in intrinsic semiconductor



Effective mass approximation

Small perturbation of periodicity: shallow impurities,
most of "hand-made" structures,
external forces

One-electron Schrödinger equation with weak and slow varying perturbation V_i (Effective mass approximation):

$$\left[\frac{p^2}{2m_0} + V(r) + V_i(r)\right]\psi(r) = E_i\psi(r)$$

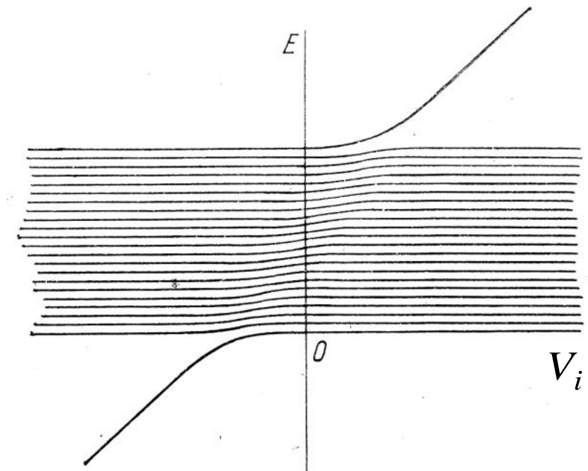
And as usual build a solution as a wave packet of Bloch wavefunctions :

$$\psi(r) = \sum_{n,k} c_n(k) e^{ikr} u_{nk}(r)$$

Bloch wave packet: $\psi(r) \approx F(r) u_0(r)$

Depending on sign of the perturbation, the top-most or bottom-most state splits from the band :

With dimensions in real and k-space $\Delta r \approx \frac{1}{\Delta k} >> a_0$



Large perturbation of periodicity → other bands need to be considered: deep impurities

Example of EMA: Hydrogen-like impurity (donor)

Hydrogen-like impurity = shallow impurity

Schrödinger equation for Hydrogen atom with effective mass and screened Coulomb potential:

$$V_i(r) = -\frac{e^2}{\varepsilon r}$$

$$\left[\frac{p^2}{2m^*} - \frac{e^2}{\varepsilon r}\right] F(r) = (E - E_C) F(r)$$

Solution for energy :

$$E_d = \frac{e^4 m^*}{2\varepsilon^2 \hbar^2} \frac{1}{n^2} = Ry \frac{m^*}{m} \frac{1}{\varepsilon^2} \frac{1}{n^2}$$

Effective Ry* :

Envelope function of the ground state :

$$F(r) = \frac{1}{(\pi a_B^3)^{1/2}} \exp\left(-\frac{r}{a_B}\right)$$

Semiconductor	Binding energy from (4.24) [meV]	Experimental binding energy of common donors [meV]
GaAs	5.72	Si_{Ga}(5.84); Ge_{Ga}(5.88) S_{As}(5.87); Se_{As}(5.79)
InP	7.14	7.14
InSb	0.6	Te_{Sb}(0.6)
CdTe	11.6	In_{Cd}(14); Al_{Cd}(14)
ZnSe	25.7	Al_{Zn}(26.3); Ga_{Zn}(27.9) F_{Se}(29.3); Cl_{Se}(26.9)

From Yu and Cordona, 2003

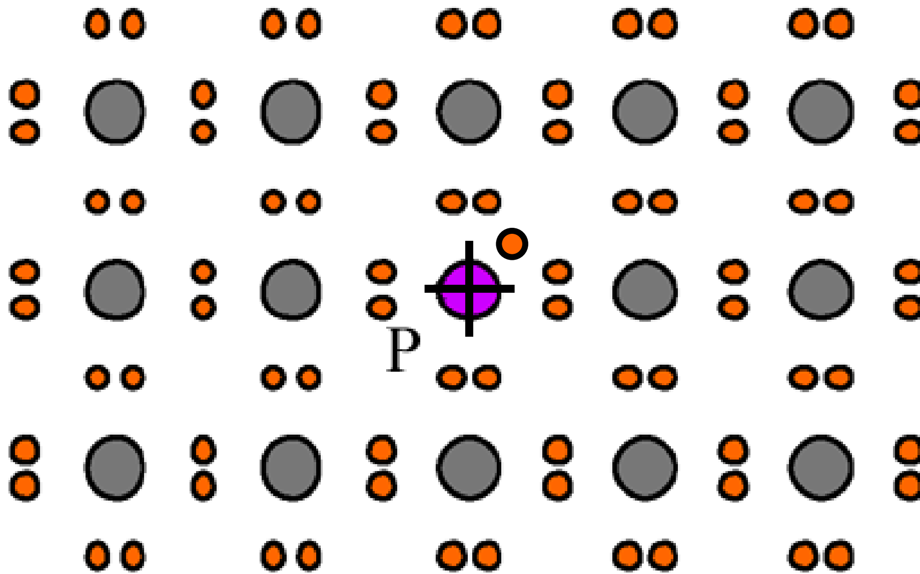
$$a_B = \frac{\hbar^2}{m_0 e^2} \frac{m_0}{m^*} \varepsilon$$

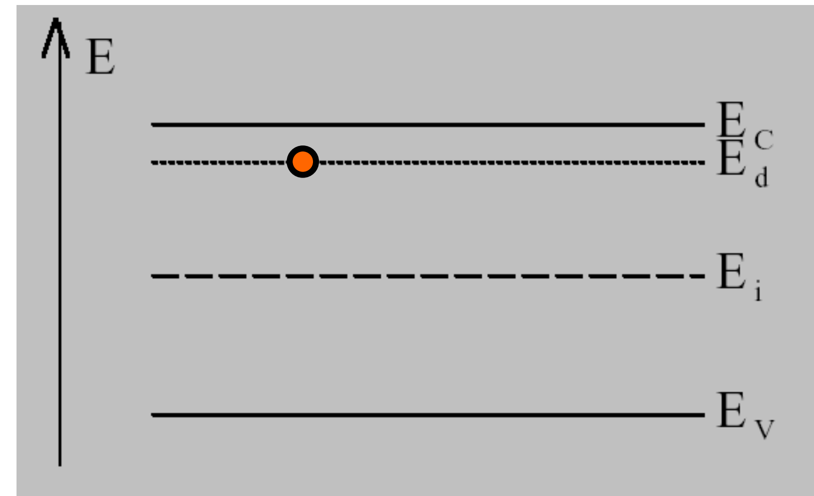
For donors in GaAs (m^*=0.07m: and $\varepsilon = 12.6$):

Ry* =6.6 meV, $a_B = 91$ A

Donors

Shallow donors:
- usually group V elements in Si and Ge (P, As, Sb)
- group IV elements on group III sublattice in III-V's (Si, Sn in GaAs)
- group VI elements on group V sublattice in III-V's (S, Te, Se in GaAs)

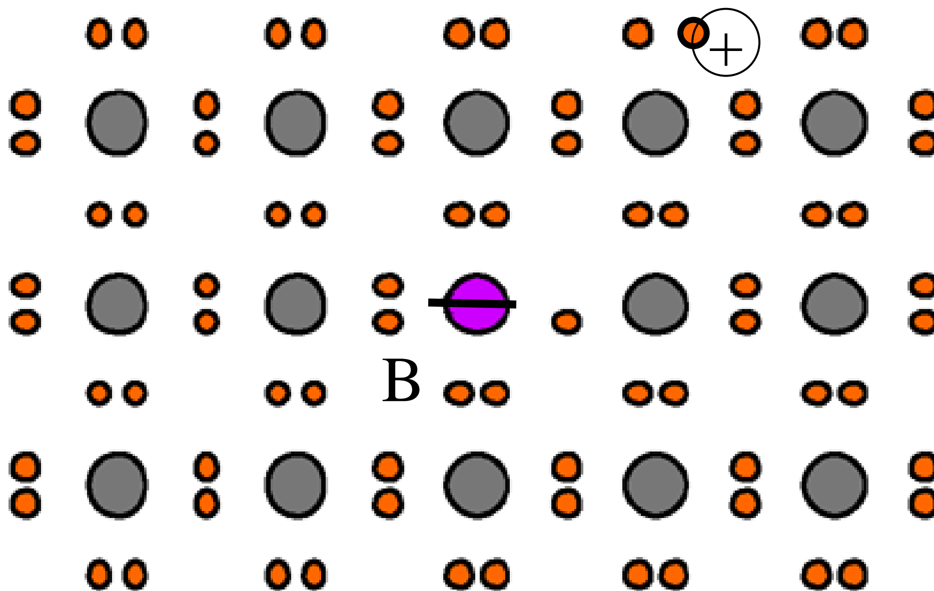


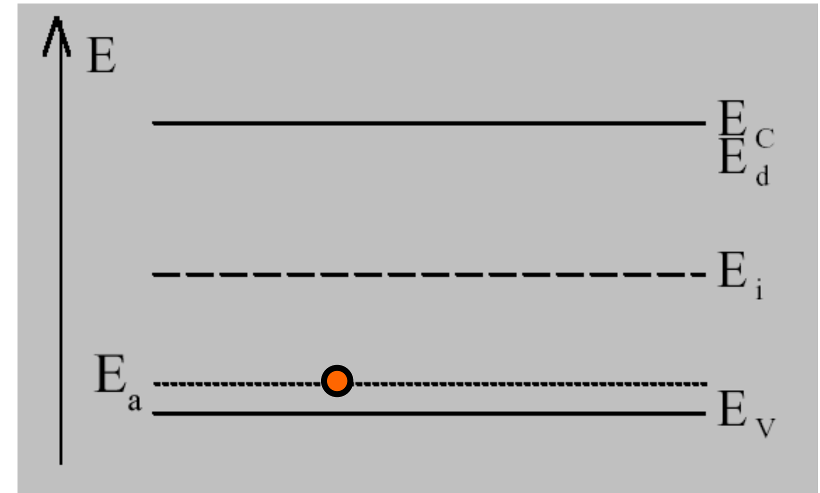


Acceptors

Shallow acceptors:
- usually group III elements in Si and Ge (B, Al, Ga, In)
- group II elements on group III sublattice in III-V's (Be, Mg, Zn in GaAs)
- group IV elements on group V sublattice in III-V's (C, Si, Ge in GaAs)

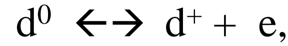
Group IV impurities in III-V's are often amphoteric.





Adding impurities: Extrinsic semiconductors

Simple impurity with two charge states, e.g. simple donor:



Total donor concentration:

$$N_d = N_d^+ + N_d^0$$

Concentration of neutral (filled with electron) and ionized donors:

$$N_d^0 = gN_d f_{FD}(E_d)$$

$$N_d^+ = N_d (1 - gf_{FD})$$

$$f_{FD}(E) = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1}$$

d^0 has a degeneracy factor *g*

Ratio of neutral to charged donors:

$$\frac{N_d^0}{N_d^+} = \frac{gf_{FD}}{1 - gf_{FD}} = ge^{\frac{E_F - E_d}{k_B T}}$$

g=2 for simple donors and
g=4 for simple acceptors

Ionization ratio for donors

$$\boxed{\frac{N_d^+}{N_d} = \frac{1}{1 + g_d e^{\frac{E_F - E_d}{k_B T}}}}$$

and acceptors:

$$\boxed{\frac{N_a^-}{N_a} = \frac{1}{1 + g_a e^{\frac{E_a - E_F}{k_B T}}}}$$

Extrinsic semiconductors: no compensation

What happens with Fermi level if semiconductors contains impurities?

In extrinsic semiconductors charge neutrality condition includes ionized impurities (instead of $n = p$ in intrinsic semiconductors):

$$n + N_a^- = p + N_d^+$$

When impurity of one type (say donors) are present:

$$n = p + N_d^+ \approx N_d^+ ; \quad if\ p << n$$

Then general equation for Fermi level (needs to be solved for degenerate semiconductors) :

$$\frac{N_d}{1 + g_d e^{\frac{E_F - E_d}{k_B T}}} = N_c \Phi_{1/2}\left(\frac{E_F - E_c}{k_B T}\right)$$

And in non-degenerate case (Δ – ionization energy):

$$\frac{N_d}{1 + g_d \frac{n}{N_c} e^{\frac{\Delta_d}{k_B T}}} = n$$

or

$$n = \frac{n_1}{2}\left(\sqrt{\frac{4N_d}{n_1} + 1} - 1\right)$$

with $n_1 = \frac{N_c}{g_d} e^{-\frac{\Delta_d}{k_B T}}$

Fermi level position (non-degenerate) using $n = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right)$

$$E_F = E_C + k_B T \ln \frac{n_1}{2N_c}\left(\sqrt{\frac{4N_d}{n_1} + 1} - 1\right)$$

Extrinsic semiconductors: no compensation

At high temperatures ($k_B T > \Delta_d$), for $\frac{4N_d}{n_1} << 1$

$$n = N_d$$

At low temperatures, for

$$\frac{4N_d}{n_1} >> 1, \quad or \quad n << N_d$$

Fermi level

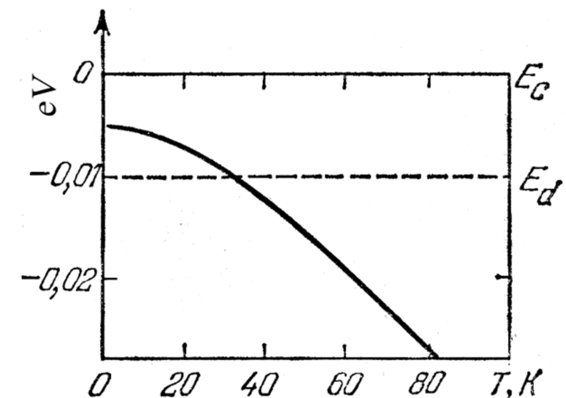
$$E_F = E_C - \frac{\Delta_d}{2} + \frac{k_B T}{2} \ln \frac{N_d}{g_d N_C}$$

and concentration

$$n = \sqrt{\frac{N_d N_C}{g_d}} e^{-\frac{\Delta_d}{2k_B T}}$$

Carriers are "freezing out"

Fermi level position in n-Ge (uncompensated)



Extrinsic semiconductors with compensation (results for a non-degenerate case)

At high temperatures, for $\frac{4(N_d - N_A)n_1}{(N_A + n_1)^2} >> 1$ and $n_1 >> N_A$

$$n = N_d - N_A$$

What is the accuracy of assumption $p << n$?

For n-type material: $n = \frac{N_d - N_a}{2} + \sqrt{\frac{(N_d - N_a)^2}{4} + n_i^2}$

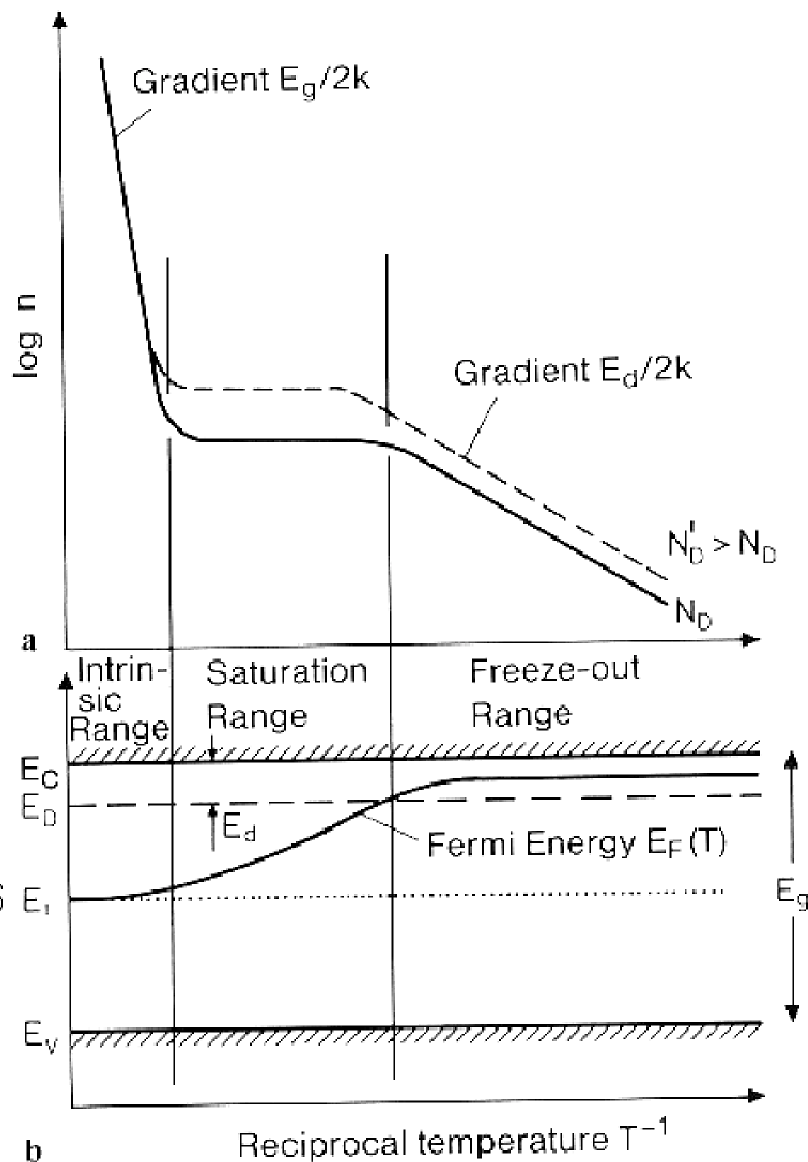
For p-type material: $p = \frac{N_a - N_d}{2} + \sqrt{\frac{(N_a - N_d)^2}{4} + n_i^2}$

At low temperatures, for $n << N_A, \quad N_d - N_A$

Fermi level $$E_F = E_d - k_B T \ln \frac{N_A}{g_d (N_d - N_A)}$$

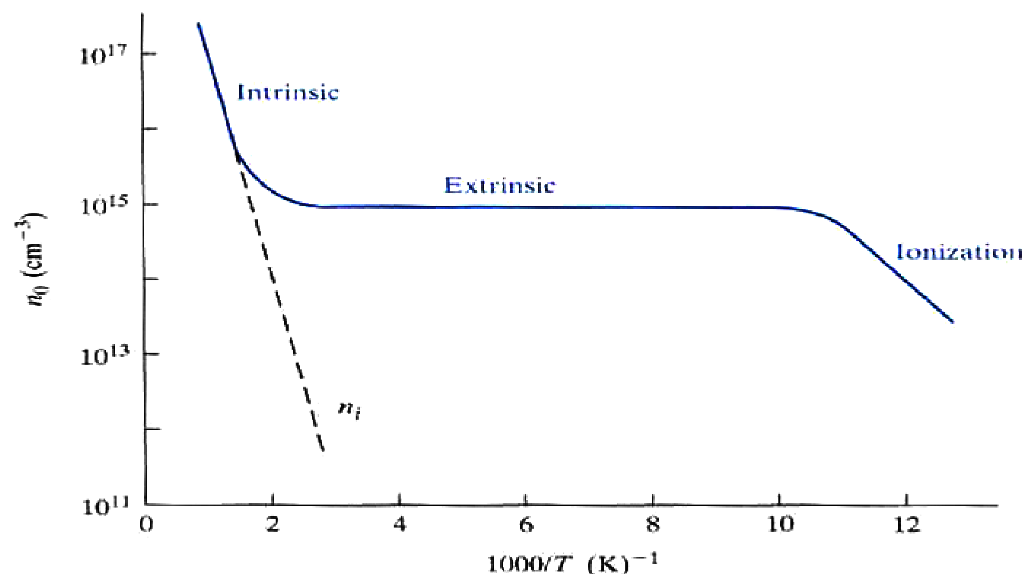
and concentration $$n = \frac{N_d - N_A}{N_A} \frac{N_C}{g_d} e^{-\frac{\Delta_d}{k_B T}}$$

Doped semiconductors: Temperature dependence



Carrier concentration vs. temperature curve has 3 distinct regions (4 regions in compensated semiconductor)

Typical dependence for Si



Strong non-degeneracy: metals again

Strong degeneracy, i.e. Fermi level lies in the conduction (or valence) band:

$$\exp\left(\frac{E_C - E_F}{k_B T}\right) << 1 \qquad or \qquad E_F > E_C$$

Carrier concentration:

$$n = N_C \Phi_{1/2}(\eta_c) \qquad \eta_c = \frac{E_F - E_C}{k_B T}$$

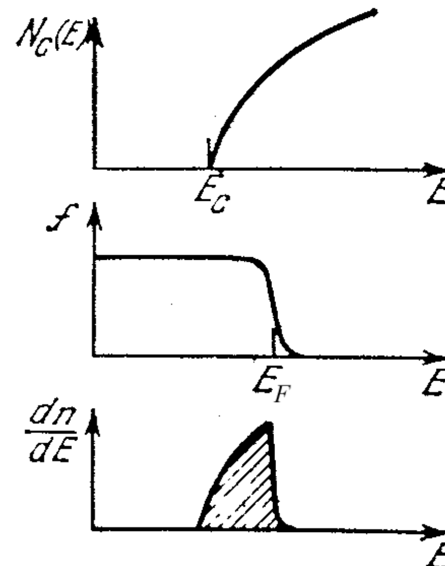
Substituting Fermi function by step function (good for $E_F - E_C > 3k_B T$)

$$n = N_C \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2} dx}{\exp(x - \eta_c) + 1} \approx N_C \frac{2}{\sqrt{\pi}} \int_0^{\frac{E_F - E_C}{k_B T}} x^{1/2} dx =$$

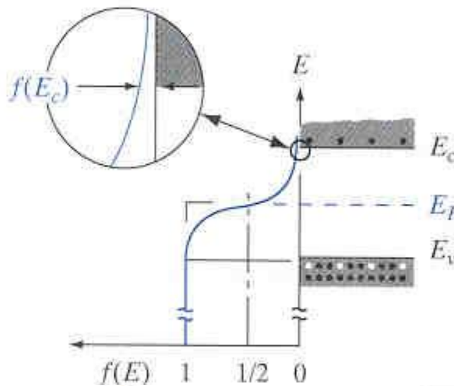
Finally:

$$n = N_C \frac{4}{3\sqrt{\pi}} \left(\frac{E_F - E_C}{k_B T}\right)^{3/2}$$

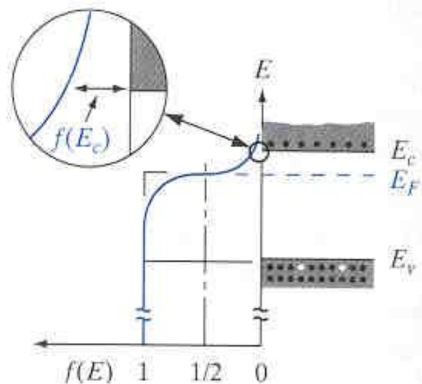
Which is similar to simple metal



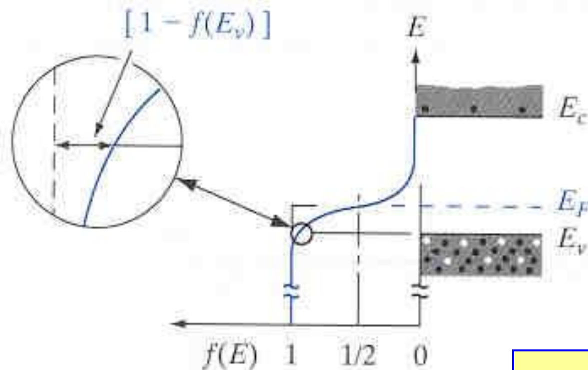
Summary of carrier statistics in semiconductors



Intrinsic



n-type



p-type

Importance of doping:

Si	Resistivity
Undoped	2×10^5 Ω-cm
Doped w/ 10^{15} As atoms/cm^3	5 Ω-cm

5 order of magnitude resistivity change due to 1 in 50 million impurities !

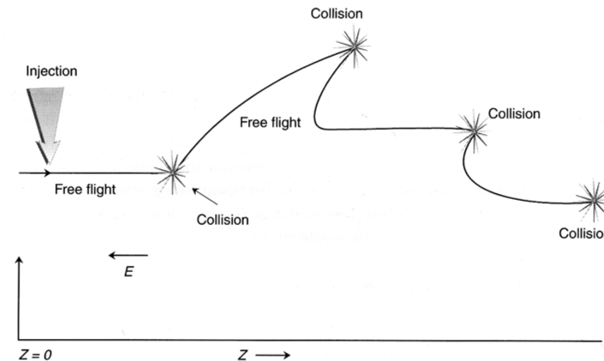
10^{15} As atoms/cm^3 in 5×10^{22} Si atoms/cm^3

- Electronic properties are extremely sensitive to impurities, defects, fields, stresses …
- Fermi level determines static carrier concentrations
- General equations can be simplified in non-degenerate and strongly degenerate cases

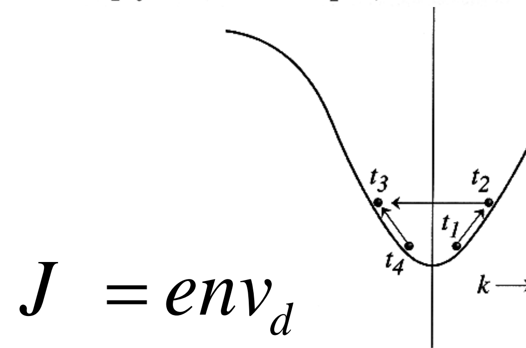
link to Java applets
http://jas.eng.buffalo.edu

Electron transport: General considerations

- Drude model again: Motion in real space = thermal motion + drift + scattering



- Motion in wavevector space: inside a band valley (unless intervalley scattering is involved)



$$J = env_d$$

- Current density is proportional to drift velocity of carriers

$$J = env_d = en\mu\mathcal{E} \equiv \sigma\mathcal{E}$$

μ –drift mobility

and gives Ohm's law:

$$\sigma = en\mu = \frac{e^2\tau_m}{m_e^*}n$$

$$\mu = \frac{e\tau_m}{m_e^*}$$

- For semiconductor containing both electron and holes:

$$\sigma = e(n\mu_e + p\mu_h)$$

Scattering mechanisms

Mathiessen's rule for relaxation time:

$$\frac{1}{\tau_m} = \frac{1}{\tau_{ac}} + \frac{1}{\tau_{op}} + \frac{1}{\tau_{ii}} + \frac{1}{\tau_{ni}} + \ldots$$

<u>In low electric fields</u>

- ionized impurities
- acoustic phonons
  - Deformation potential
  - Piezoelectric

<u>In high electric fields</u>

- optical phonons
- intervalley scattering

<u>At high concentrations</u>

- carrier-carrier scattering

To understand how these mechanisms affect mobility one needs to consider dependence $\tau(E)$

Conductivity effective mass

- For non-degenerate conduction band minimum (Γ-point):

$$m_e^* = m_\Gamma$$

- Indirect conduction band minimum: effective mass will depend on direction!
  - For example: Si along [100] direction: $$J_n = J_{ex} + J_{ey} + J_{ez} = \left(2\frac{n}{6}\frac{e^2\tau_m}{m_l} + 2\cdot 2\frac{n}{6}\frac{e^2\tau_m}{m_t} \right)\varepsilon$$
  - Conductivity effective mass of Si [100] electrons:: $$\frac{1}{m_c^*} = \frac{1}{3}\left(\frac{1}{m_l} + \frac{2}{m_t} \right)$$

- Valence band maximum: need to add up contributions of light and heavy holes: $$J_p = J_{lh} + J_{hh} = \left(\frac{p_{lh}}{m_{lh}} + \frac{p_{hh}}{m} \right) e^2 \tau_{mh} \varepsilon$$

- Conductivity effective mass of holes $$\frac{1}{m_v^*} = \frac{1}{p}\left(\frac{p_{lh}}{m_{lh}} + \frac{p_{hh}}{m_{hh}} \right) = \frac{m_{lh}^{1/2} + m_{hh}^{1/2}}{m_{lh}^{3/2} + m_{hh}^{3/2}}$$

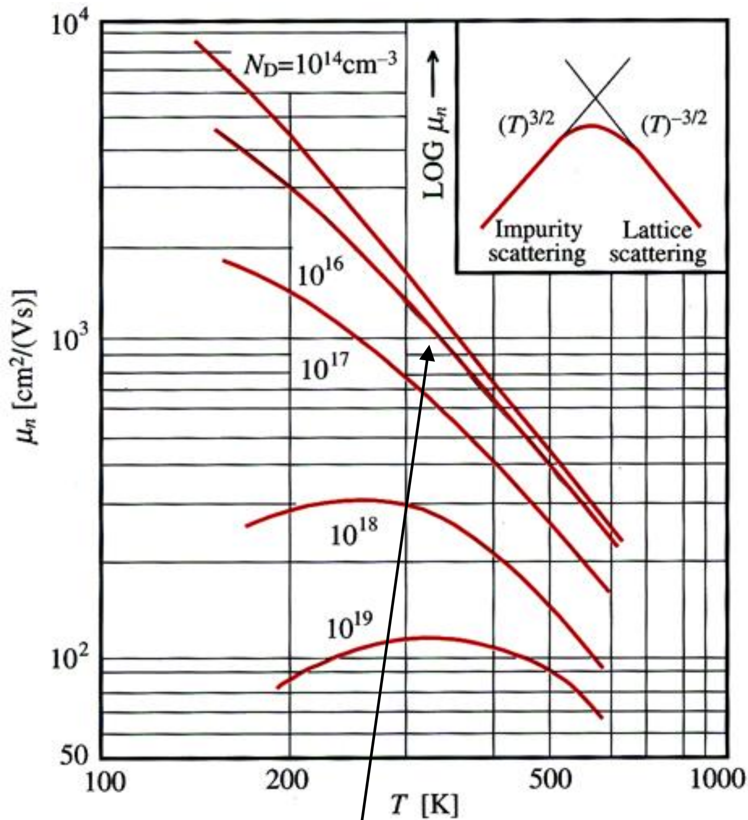
Effective masses and low field mobilities at room temperature:

	a (Å)	ε_r (rel.)	ρ (g/cm $^{-3}$)	E_g (eV)	m_n	m_p	μ_n (cm ^{2}/Vs)	μ_p (cm ^{2}/Vs)
Si	5.43	11.8	2.33	1.12	1.08	0.56	1350	480
Ge	5.66	16.0	5.32	0.67	0.55	0.37	3900	1900
GaAs	5.65	13.2	5.31	1.42	0.067	0.48	8500	400
InP	5.87	12.1	4.79	1.35	0.080	–	4000	100

Temperature dependence of mobility

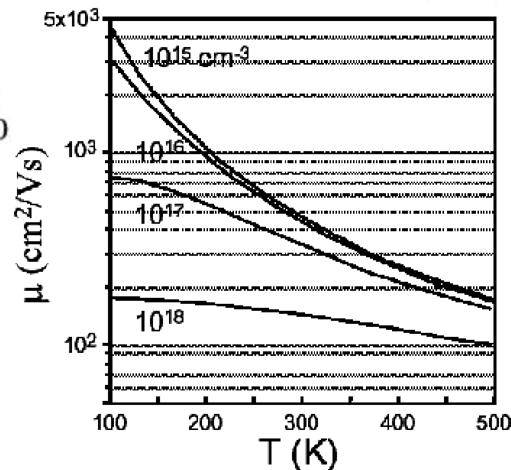
Relaxation time τ_m depends on energy!

Mobility in n-Si

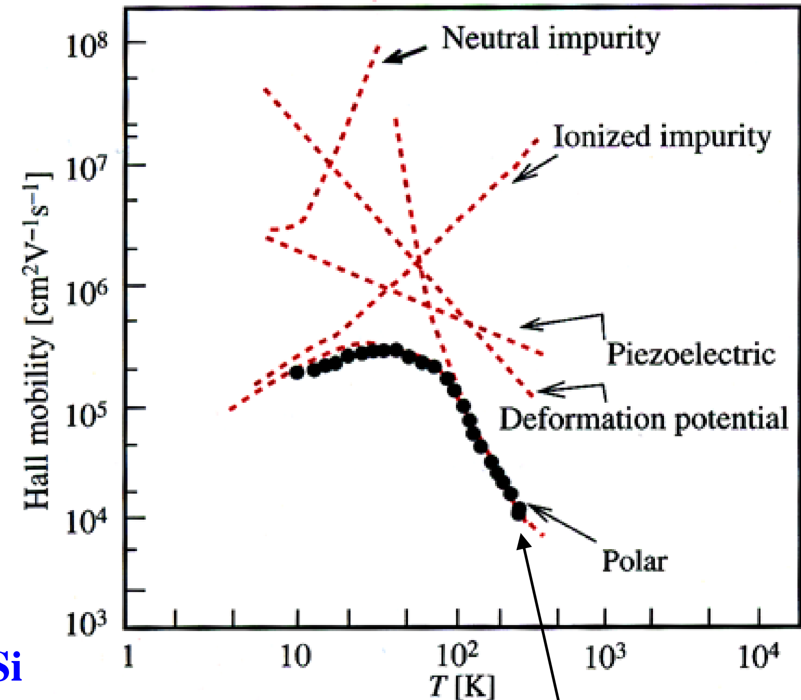


Intravalley acoustic phonon scattering + (2TA+LO) intervaley phonon scattering

Mobility in p-Si



Mobility in n-GaAs



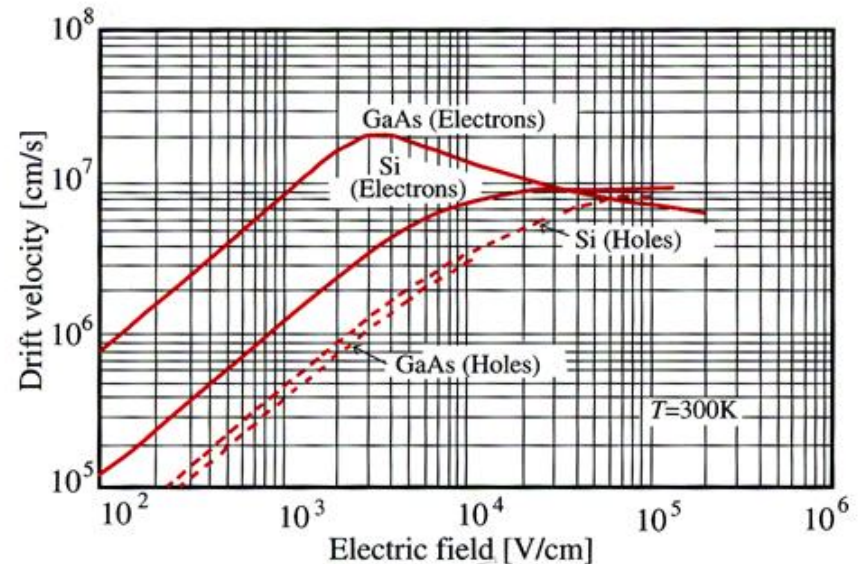
LO phonon scattering

From Yu and Cordona, 2003, and Shur, 2003

High field electron transport

Hot electrons transfer energy into thermal vibrations of the crystal lattice (phonons). Such vibrations can be modeled as harmonic oscillations with a certain frequency, ω_{ph} . The energy levels of a harmonic oscillator are equidistant with the energy difference between the levels equal to

$$E_{ph} = \hbar\omega_{ph}$$



Two types of phonons scatter electrons differently: acoustical (slow) and optical (fast):

$$E_{ac} = \hbar\omega_{ac} \approx kT$$

$$E_{opt} = \hbar\omega_{opt} \approx 40meV$$

Hence, process for a hot electron can be represented as follows. The electron accelerates in the electric field until it gains enough energy to excite optical phonon:

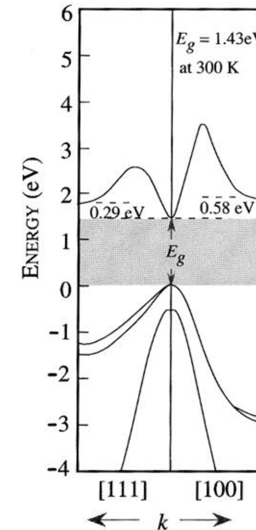
Intervalley scattering in high electric field

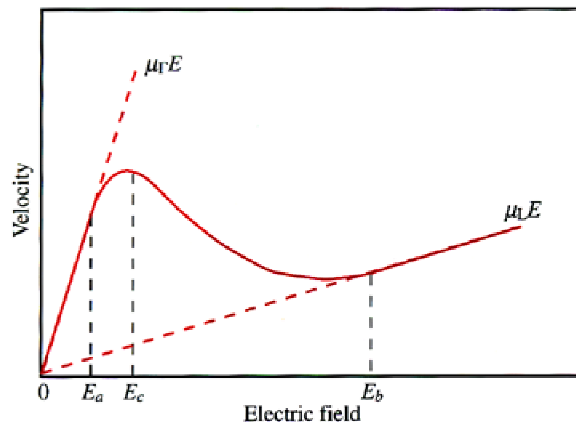
GaAs has an L valley just 0.29 eV higher than Γ -valley

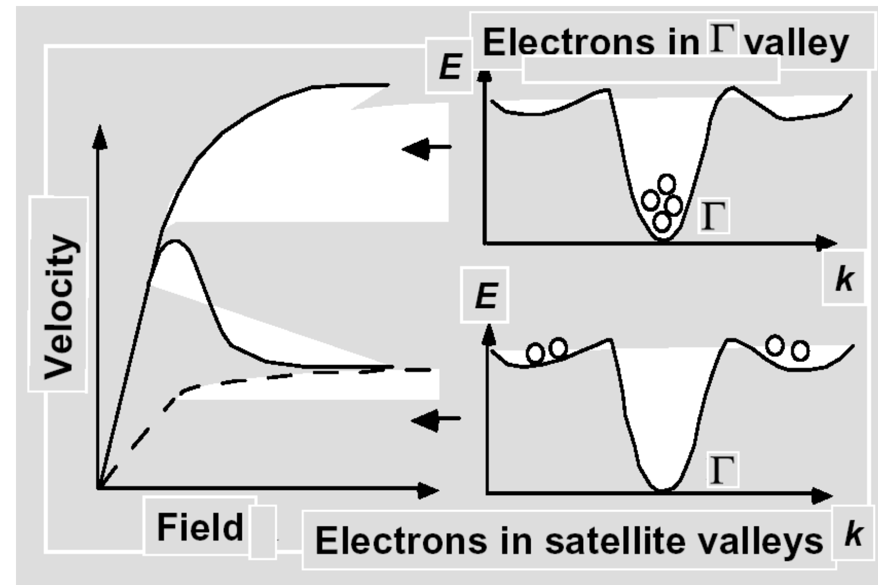
At high fields electrons can be transferred into L-valleys. The conductivity will depend on concentrations and mobilities of electrons in both valleys:

$$\sigma = e(N_\Gamma \mu_\Gamma + N_L \mu_L)$$

Model for dependence of drift velocity on electric field in GaAs







From Shur, 2003

Diffusion and drift of carriers

- If we increase or decrease carrier concentration in some region of a sample, the carriers will tend to diffuse to return to equilibrium
- Diffusion is described by the first Fick's law:

(Flux of particles)= -(Diffusion coef.) x (gradient of concentration)

Electron diffusion current $$J_n = eD_n \nabla n$$

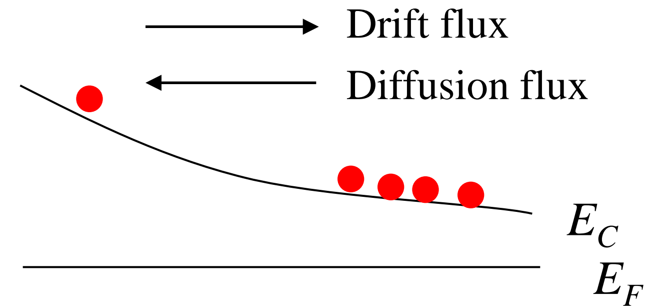
Hole diffusion current $$J_p = -eD_p \nabla p$$

- If electric field (weak) is applied:

Total electron current $$J_n = ne\mu_n \mathcal{E} + eD_n \nabla n$$

Total hole current $$J_p = pe\mu_o \mathcal{E} - eD_p \nabla p$$

Einstein relation



At equilibrium condition (no total current) diffusion current is equal to drift current:

$$ne\mu_n\mathcal{E} + eD_n\nabla n = 0$$

For nondegenerate semiconductor: $$n = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right)$$

Carrier concentration is changing in the electric field $\phi(r)$:

$$n(x) = n_0 \exp\left(\frac{e\varphi(x)}{k_B T}\right)$$

Gradient of electron concentration is : $$\nabla n = n\frac{e}{k_B T}\nabla\varphi(x) = n\frac{e}{k_B T}\mathcal{E}$$

And substituting, obtain Einstein relation: $$D = \frac{k_B T}{e}\mu$$

$$\mu = \frac{e\tau_m}{m_e^*}$$