Physics of Semiconductors
Physik von Halbleitern

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Automn Semester 2014

Literature: S.M. Sze, The Physics of Semiconductor Devices

Physics of Semiconductors

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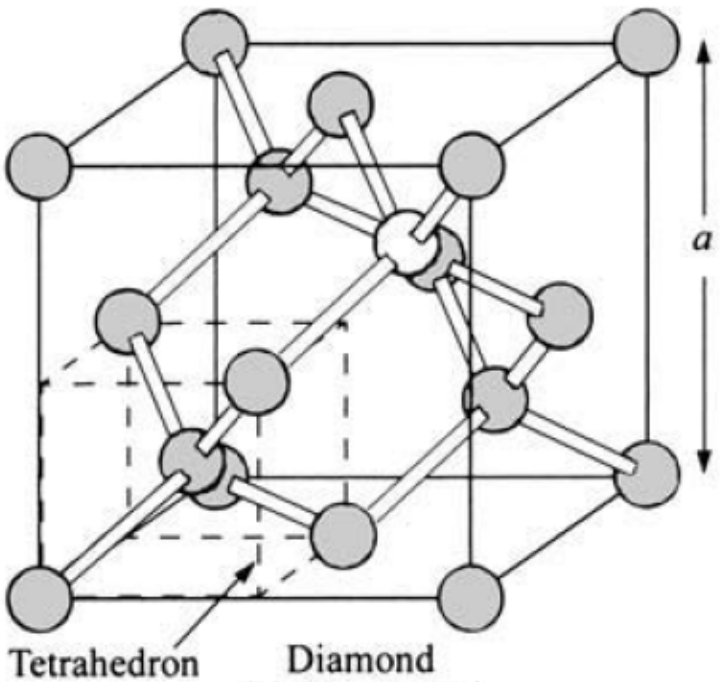
Tuesday 10-12 in HS 1, Department of Physics

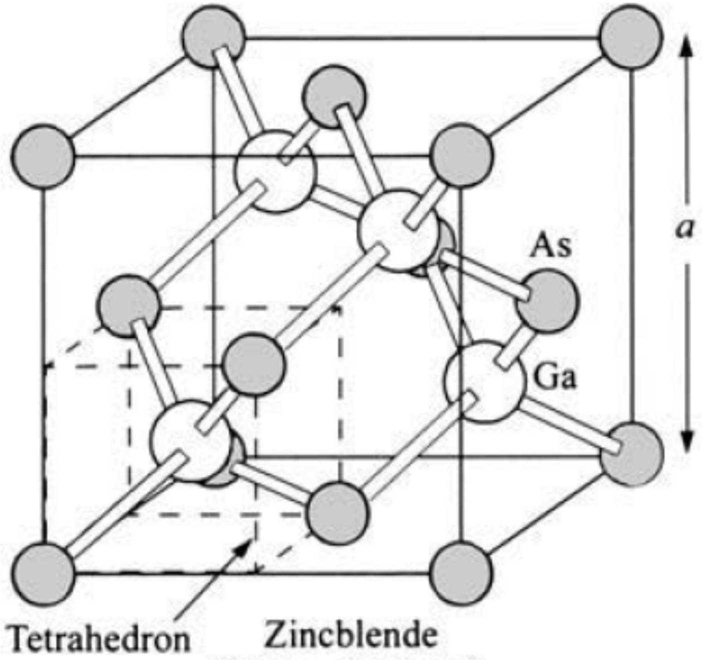
Contents:

16.9.	Introduction to Semiconductors (EM)
23.9.	p-n Junctions (EM)
30.9.	Metal-Semiconductor Contacts (EM)
7.10.	Metal-Insulator-Semiconductor Contacts (EM)
14.10.	Bipolar Transistors (EM)
21.10.	MOSFETS (EM)
28.10.	Power Devices I (HB)
4.11.	Power Devices II (HB)
11.11.	LED and Lasers (TG)
18.11.	Photodectors and Solar Cells (TG)
25.11.	Photodectors and Solar Cells (TG)
2.12.	Sensors (EM)
9.12.	Summary/Questions/Preparation (EM/TG)
16.12.	Exam

Crystal structures:
Diamond and Zincblende



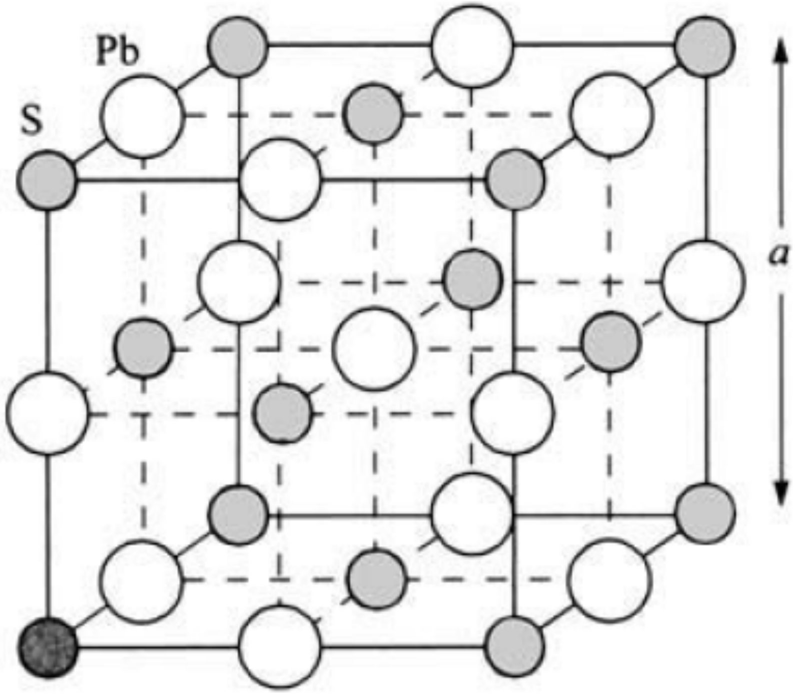
Diamond
(Si, Ge, C, etc.)



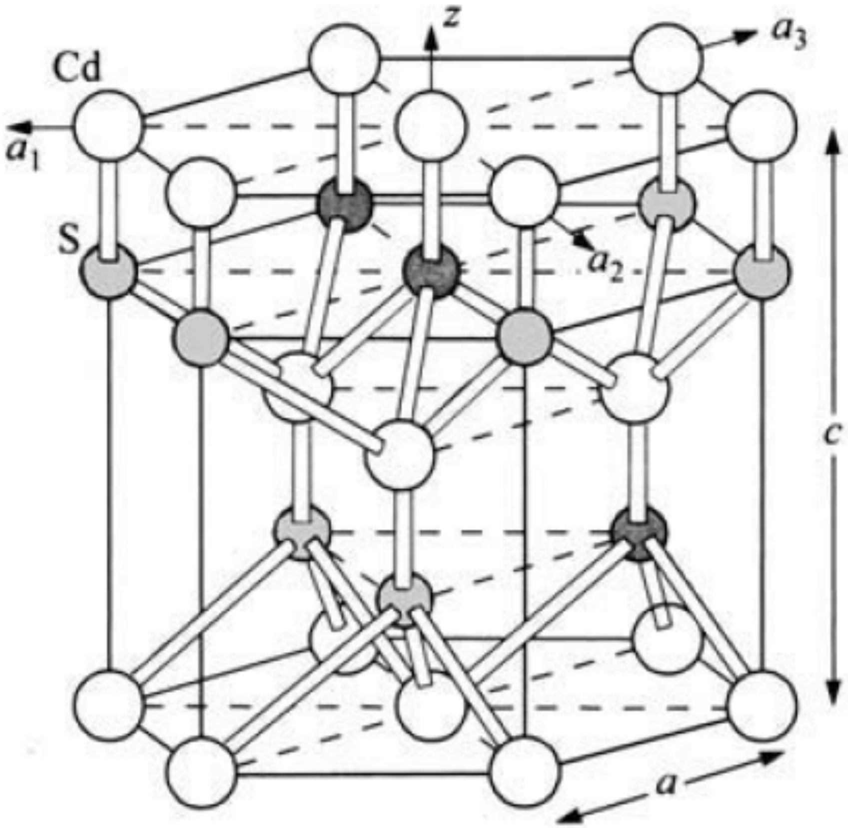
Zincblende
(GaAs, GaP, etc.)

Can be created by two fcc-lattices: 2 Si for silicon or Ga and As-sublattice for GaAs

Rock salt and Wurtzite structures

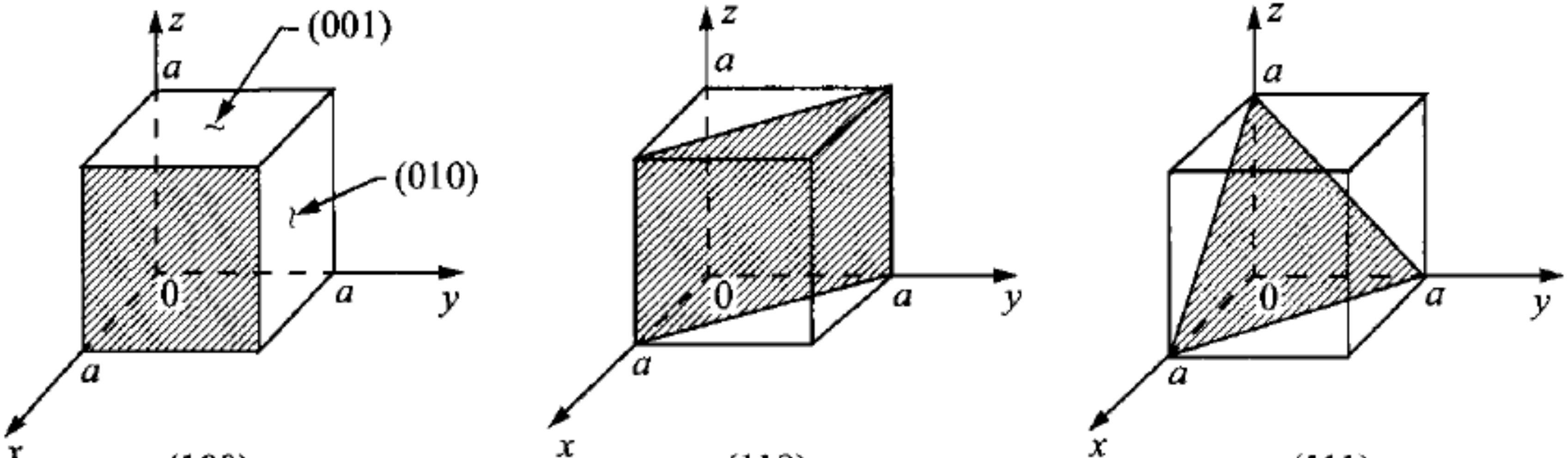


Rock-salt
(PbS, PbTe, etc.)

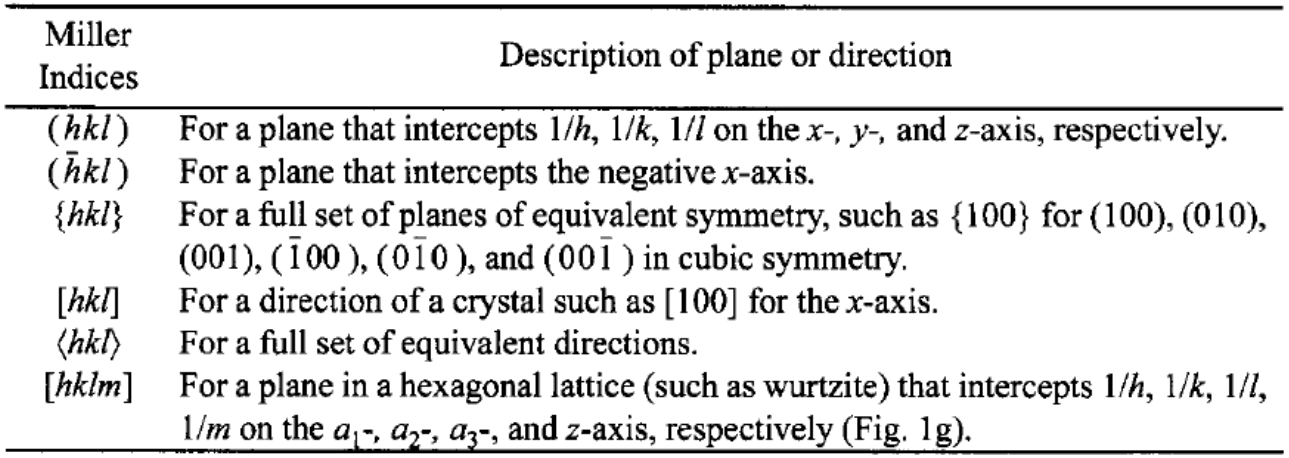


Wurtzite
(CdS, ZnS, etc.)

Miller indices



(100) (110) (111)



Miller Indices	Description of plane or direction
(hkl)	For a plane that intercepts $1/h$, $1/k$, $1/l$ on the x-, y-, and z-axis, respectively.
$(\bar{h}kl)$	For a plane that intercepts the negative x-axis.
$\{hkl\}$	For a full set of planes of equivalent symmetry, such as {100} for (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, and $(00\bar{1})$ in cubic symmetry.
$[hkl]$	For a direction of a crystal such as [100] for the x-axis.
$\langle hkl\rangle$	For a full set of equivalent directions.
$[hklm]$	For a plane in a hexagonal lattice (such as wurtzite) that intercepts $1/h$, $1/k$, $1/l$, $1/m$ on the a_1-, a_2-, a_3-, and z-axis, respectively (Fig. 1g).

Reciprocal lattice

Direct lattice: $\boldsymbol{R} = m\boldsymbol{a} + n\boldsymbol{b} + p\boldsymbol{c}$

Reciprocal lattice: $\boldsymbol{G}\cdot\boldsymbol{R} = 2\pi \times \text{Integer}$

Reciplocal lattic vectors are perpendicular to set of planes in the direct lattice and can be constructed from the unit cell vectors of the direct lattice

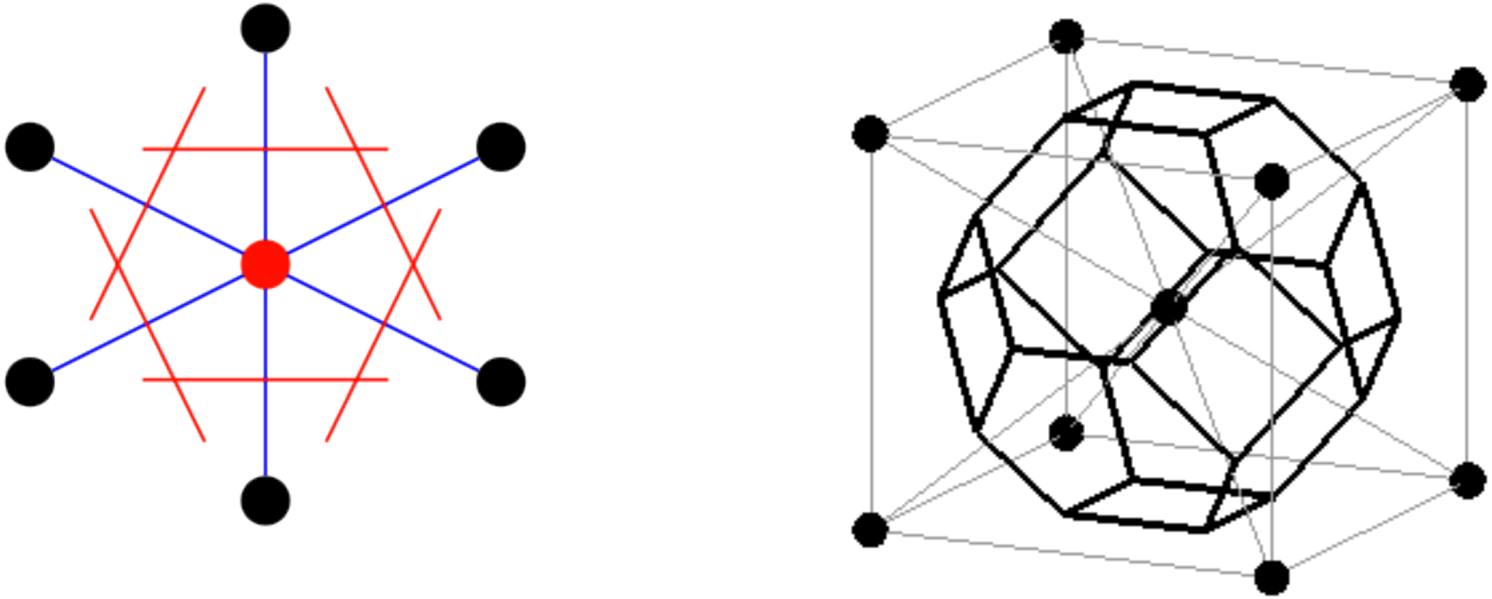
$$\boldsymbol{a}^* \equiv 2\pi\frac{\boldsymbol{b}\times\boldsymbol{c}}{\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c}} \qquad \boldsymbol{c}^* \equiv 2\pi\frac{\boldsymbol{a}\times\boldsymbol{b}}{\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c}}$$

$$\boldsymbol{b}^* \equiv 2\pi\frac{\boldsymbol{c}\times\boldsymbol{a}}{\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c}}$$

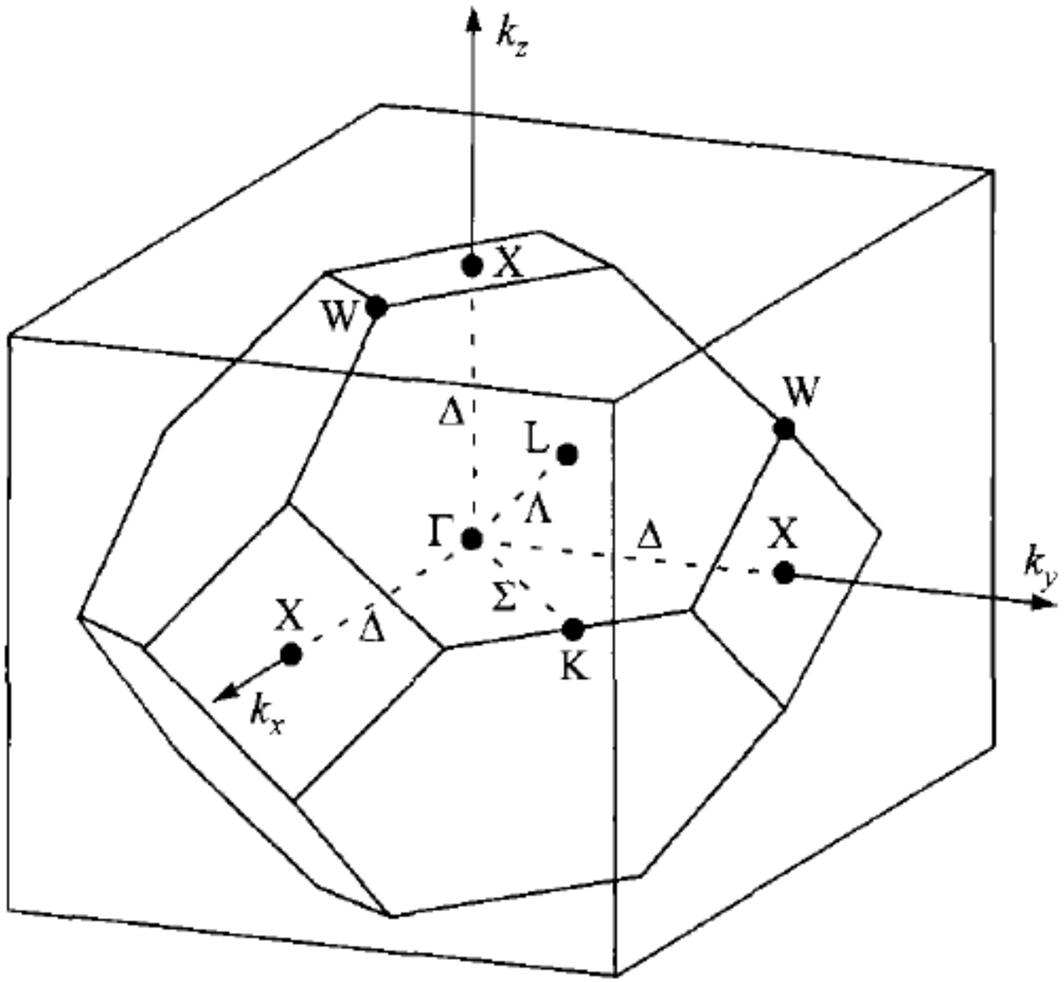
Reciprocal lattice: $\boldsymbol{G} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$

Wigner-Seitz cell and Brillouin zone

Wigner-Seitz cells are constructed by the bisector planes



Brillouin zone of fcc-lattice and diamond lattice



The Brillouin zone is the Wigner-Seitz cell of the Reciprocal lattice

Example:
Direct lattice: fcc with a
Reciprocal lattice: bcc with 4pi/a
Wigner-Seitz of reciprocal lattice is truncated octahedron and corresponds to the Brillouin zone

Brillouin zone of fcc

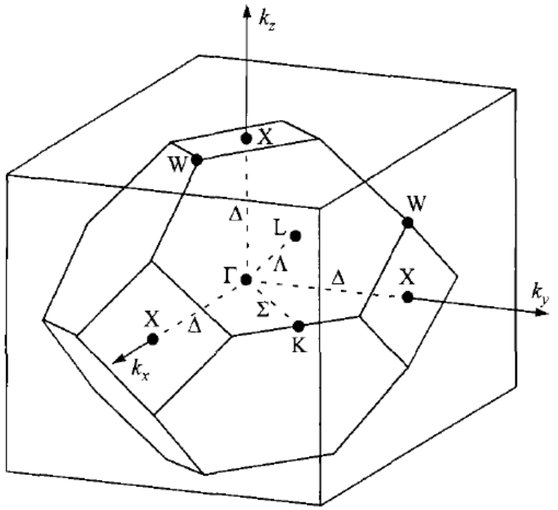


Table 2 Brillouin Zone of fcc, Diamond, and Zincblende Lattices: Zone Edges and Their Corresponding Axes (Γ is the Center)

Point	Degeneracy	Axis
Γ, (0,0,0)	1	
X, $2\pi/a(\pm1,0,0)$, $2\pi/a(0,\pm1,0)$, $2\pi/a(0,0,\pm1)$	6	Δ, ⟨1,0,0⟩
L, $2\pi/a(\pm1/2,\pm1/2,\pm1/2)$	8	Λ, ⟨1,1,1⟩
K, $2\pi/a(\pm3/4,\pm3/4,0)$, $2\pi/a(0,\pm3/4,\pm3/4)$, $2\pi/a(\pm3/4,0,\pm3/4)$	12	Σ, ⟨1,1,0⟩

Bloch theorem and Band structure

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r},\boldsymbol{k}) = E(\boldsymbol{k})\psi(\boldsymbol{r},\boldsymbol{k})$$

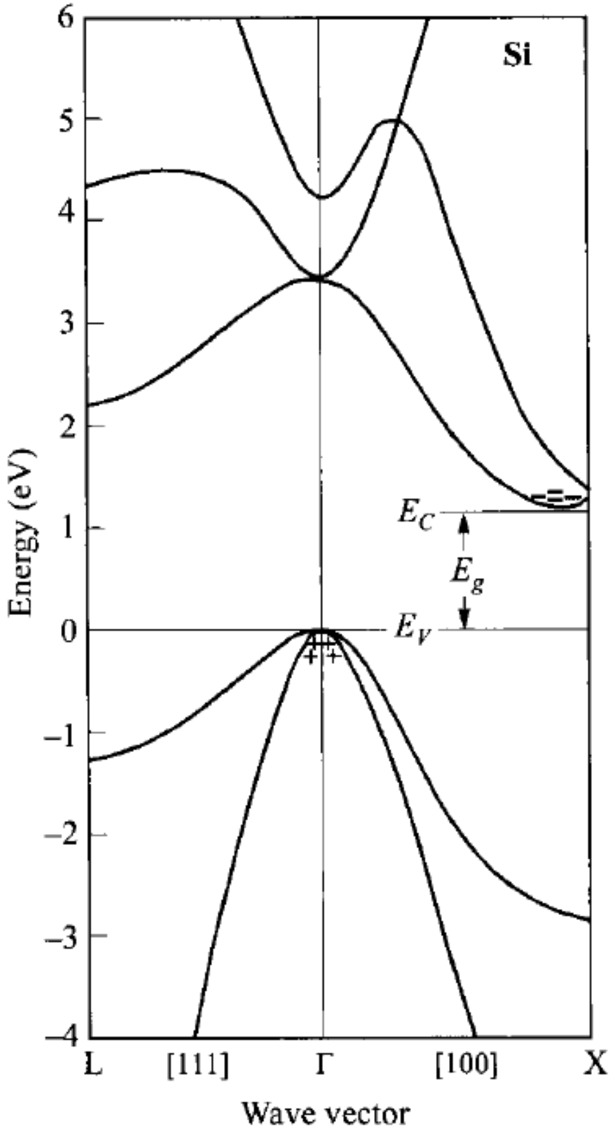
The solution of the Schrödinger-Equation for a periodic potential V(r)=V(r+R) are Bloch states:

$$\psi(\boldsymbol{r},\boldsymbol{k}) = \exp(j\boldsymbol{k}\cdot\boldsymbol{r})U_b(\boldsymbol{r},\boldsymbol{k}).$$

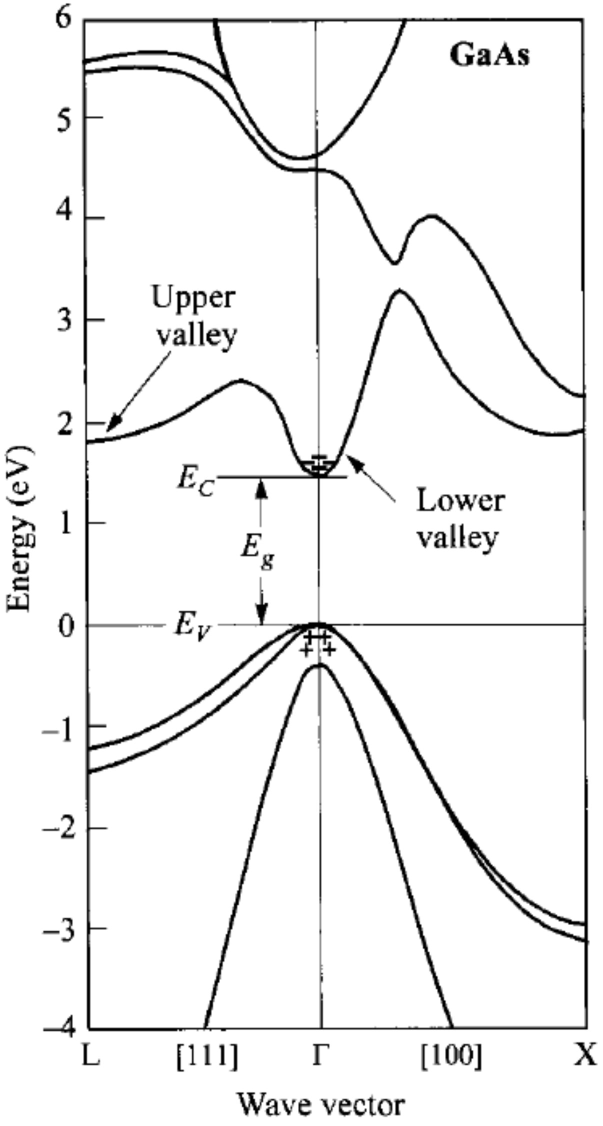
Ub(r)=Ub(r+R) is periodic and k has to fulfill kR=2pi
which is true for the reciprocal vectors G

The energy E is also periodic in G and it is sufficient to describe E(k)
in the Brillouin zone

E(k) for Silicon and GaAs



indirect sc

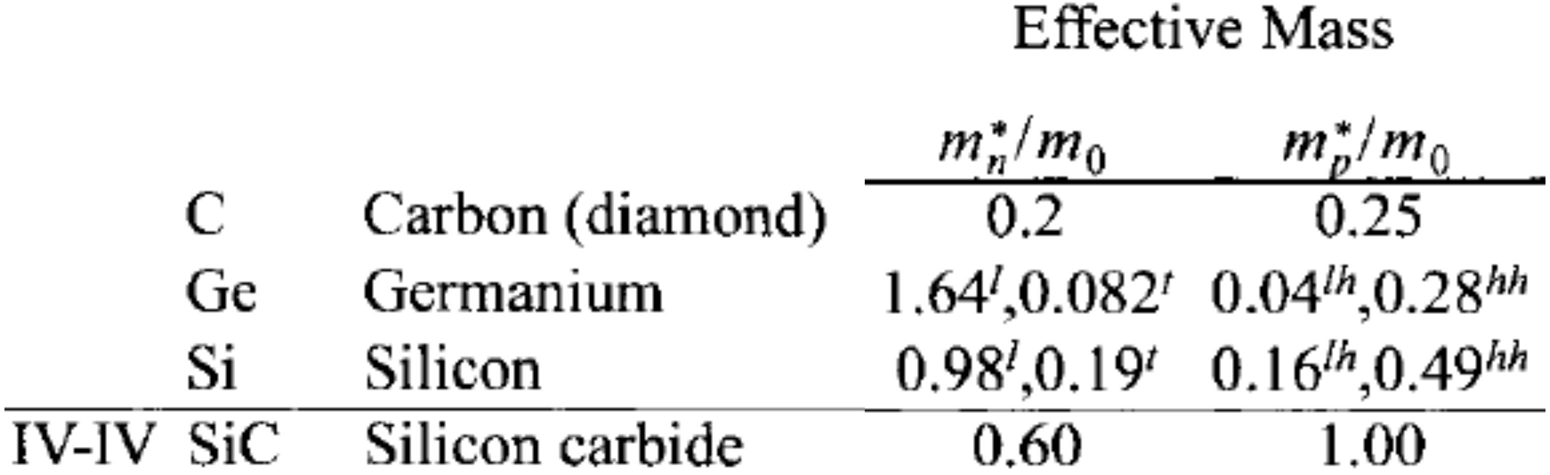


direct sc

Effektive masses

Near the bottom of the conduction band and top of valence band, one can approximate the bands by parabola of different curvatures (light and heavy electrons and light and heavy holes)

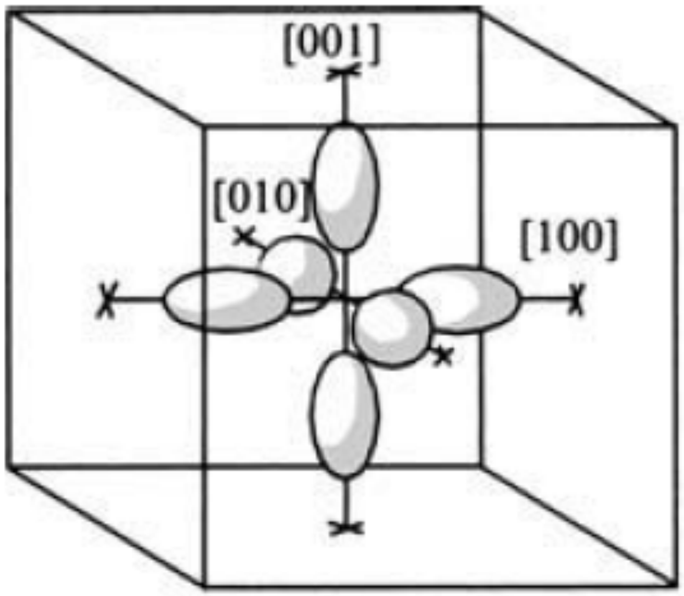
$$E(k) = \frac{\hbar^2 k^2}{2m^*} \quad \text{where} \quad \frac{1}{m^*_{ij}} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E(k)}{\partial k_i \partial k_j}$$



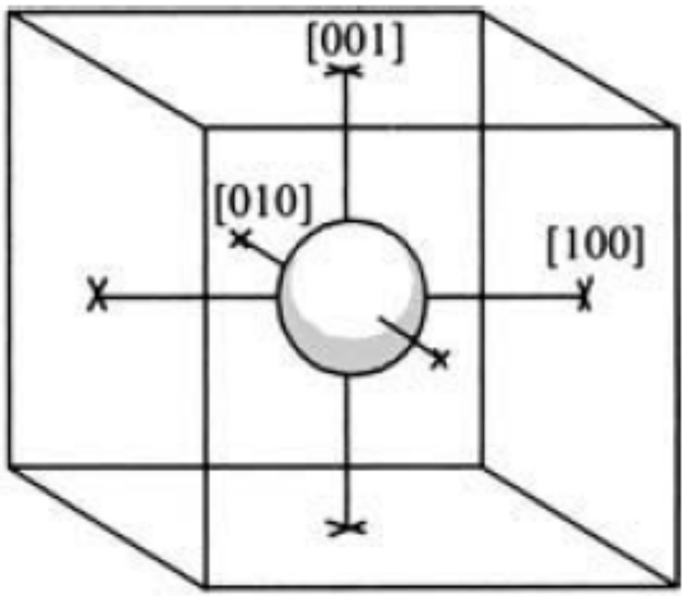
Effective Mass

			m_n^*/m_0	m_p^*/m_0
	C	Carbon (diamond)	0.2	0.25
	Ge	Germanium	$1.64^l, 0.082^t$	$0.04^{lh}, 0.28^{hh}$
	Si	Silicon	$0.98^l, 0.19^t$	$0.16^{lh}, 0.49^{hh}$
IV-IV	SiC	Silicon carbide	0.60	1.00

Shapes for constant energy surfaces for Si and GaAs

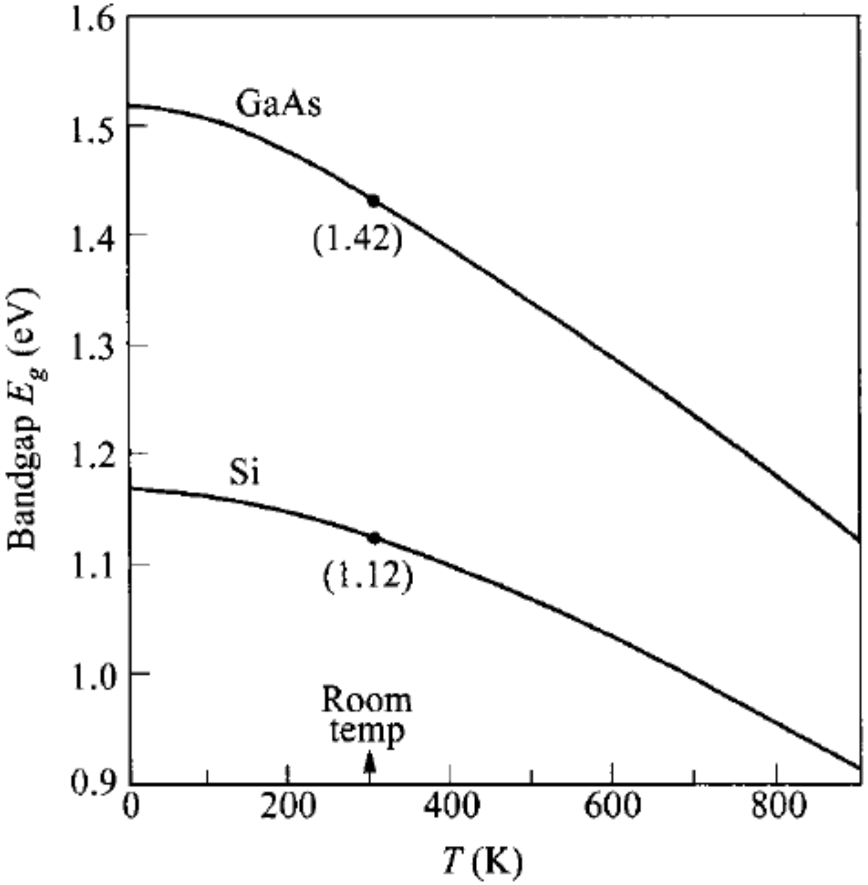


Si



GaAs

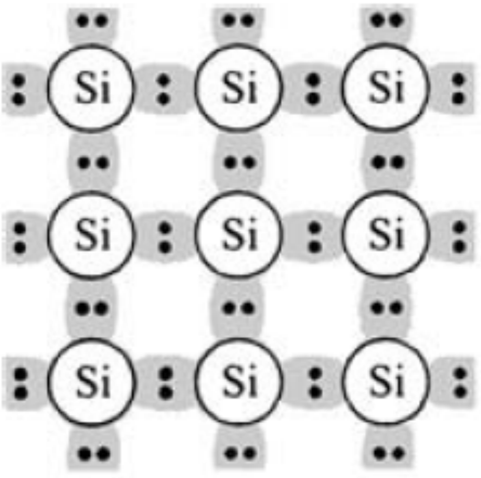
Gap energy as a function of temperature



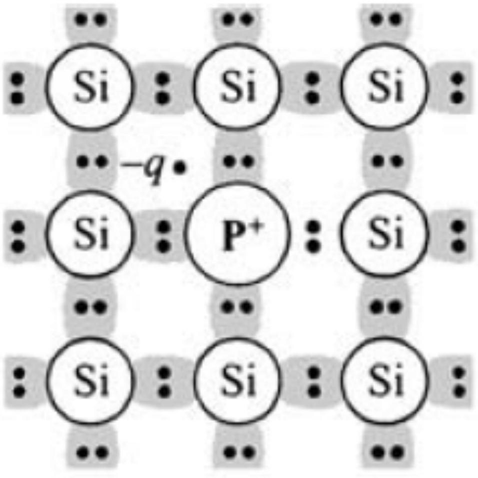
	$E_g(0)$ (eV)	α (eV/K)	β (K)
GaAs	1.519	5.4×10^{-4}	204
Si	1.169	4.9×10^{-4}	655

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

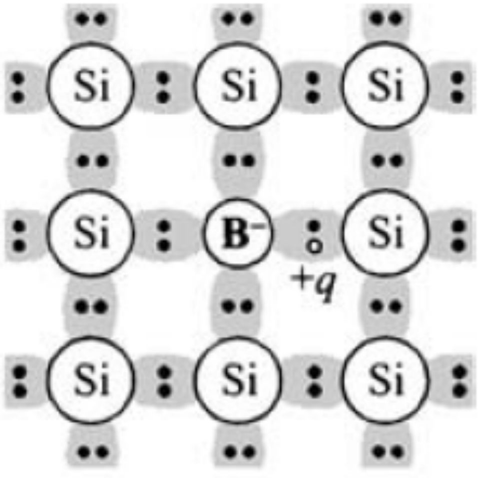
Charge carriers in sc



Intrinsic sc



n-doped silicon
with donor P
=> electron conductor



p-doped
with acceptor B
=> hole conductor

Carrier concentrations (intrinsic)

$$n = \int_{E_C}^{\infty} N(E)F(E)dE \quad \Rightarrow \quad n = N_C \exp\left(-\frac{E_C - E_F}{kT}\right)$$

$$F(E) = \frac{1}{1 + \exp[(E - E_F)/kT]}$$

or

$$E_C - E_F = kT \ln\left(\frac{N_C}{n}\right)$$

$$N(E) = M_C \frac{\sqrt{2}}{\pi^2} \frac{m_{de}^{3/2}(E - E_C)^{1/2}}{\hbar^3}$$

$$N_C \equiv 2\left(\frac{2\pi m_{de} kT}{h^2}\right)^{3/2} M_C$$

$$m_{de} = (m_1^* m_2^* m_3^*)^{1/3}$$

Non-generate case (doping smaller than Nc) => Boltzmann statistics

Carrier concentrations (intrinsic)

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

$$N_V \equiv 2\left(\frac{2\pi m_{dh} kT}{h^2}\right)^{3/2}$$

$$m_{dh} = ({m^*_{lh}}^{3/2} + {m^*_{hh}}^{3/2})^{2/3}$$

Effective density of states

$$N_C = 2\cdot\left(2\pi\cdot k_B\cdot T\cdot\frac{m_e^*}{h^2}\right)^{3/2}$$

$$N_C = 2.5\left(\frac{m_e^*}{m_e}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2}\times 10^{19}\,\mathrm{cm}^{-3}$$

$$N_V = 2\cdot\left(2\pi\cdot k_B\cdot T\cdot\frac{m_h^*}{h^2}\right)^{3/2}$$

$$N_V = 2.5\left(\frac{m_h^*}{m_e}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2}\times 10^{19}\,\mathrm{cm}^{-3}$$

Carrier concentrations (intrinsic)

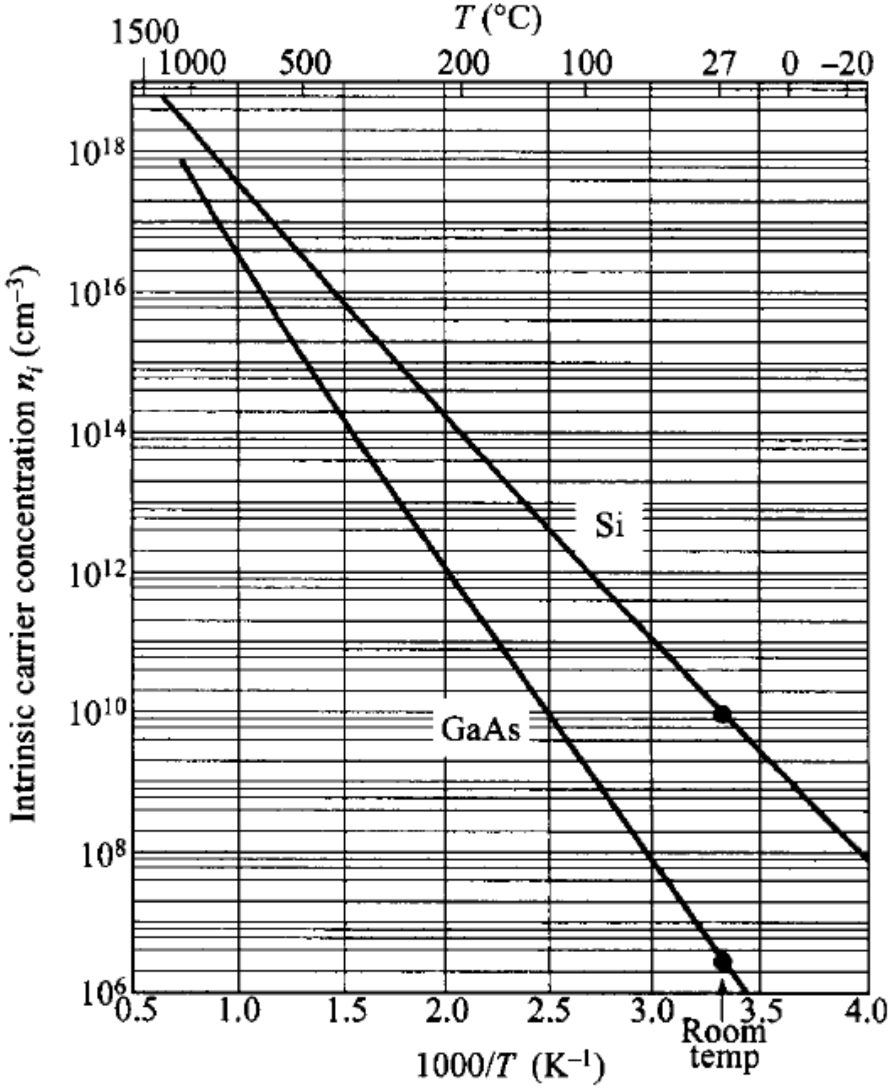
$p=n=n_i$ Thermal excitation from valence band to conduction band leads to charge carrieres => n=p

$$E_F = E_i = \frac{E_C+E_V}{2} + \frac{kT}{2}\ln\left(\frac{N_V}{N_C}\right)$$
$$= \frac{E_C+E_V}{2} + \frac{3kT}{4}\ln\left(\frac{m_{dh}}{m_{de}M_C^{2/3}}\right)$$

Fermi level lies close
to the middle of the gap,
but not exactly

$$n_i = N_C\exp\left(-\frac{E_C-E_i}{kT}\right) = N_V\exp\left(-\frac{E_i-E_V}{kT}\right) = \sqrt{N_C N_V}\exp\left(-\frac{E_g}{2kT}\right)$$
$$= 4.9\times10^{15}\left(\frac{m_{de}m_{dh}}{m_0^2}\right)^{3/4} M_C^{1/2}T^{3/2}\exp\left(-\frac{E_g}{2kT}\right) \quad .$$

Intrinsic carrier density n_i



Si: n_i=9.65 10^9cm^{-3}

GaAs: n_i=2.1 10^6cm^{-3}

Mass action law

$$\begin{aligned} pn &= N_C N_V \exp\left(-\frac{E_g}{kT}\right) \\ &= n_i^2 \quad , \end{aligned}$$

Also valid for doped material (non-degenerate case)

Donor and Acceptor levels

cf. Hydrogen atom:

$$E_H = \frac{m_0 q^4}{32\pi^2 \varepsilon_0^2 \hbar^2} = 13.6\ \text{eV}$$

Ionisation energy is:

$$E_C - E_D = \left(\frac{\varepsilon_0}{\varepsilon_s}\right)^2 \left(\frac{m_{ce}}{m_0}\right) E_H$$

$$m_{ce} = 3\left(\frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*}\right)^{-1}$$

=> 0.025eV for Si and 0.007eV for GaAs

Ionization is usually complete at RT $N_D^+ \approx N_D$

Calculation of ionization level

$$N_D^+ = \frac{N_D}{1 + g_D \exp[(E_F - E_D)/kT]}$$

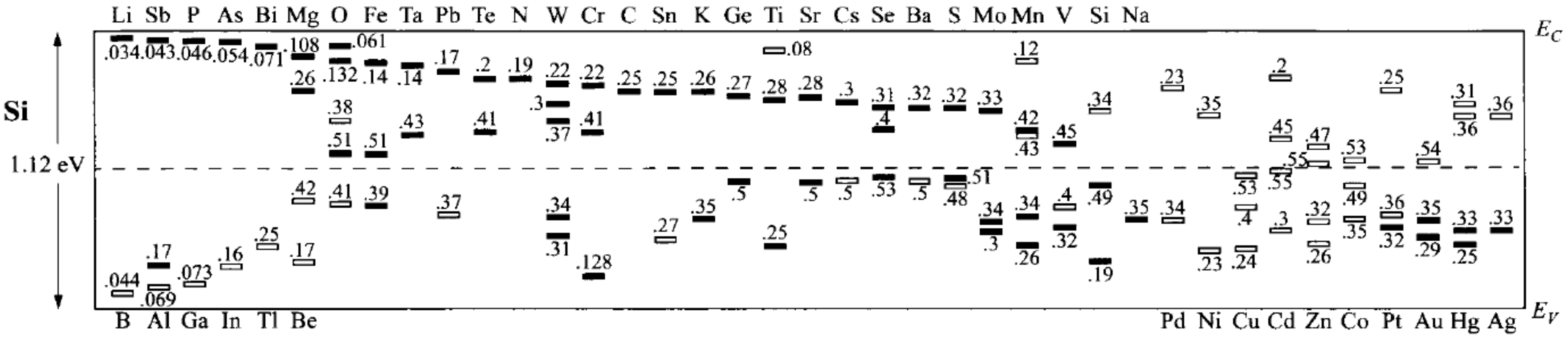
$g_D=2$

$$N_A^- = \frac{N_A}{1 + g_A \exp[(E_A - E_F)/kT]}$$

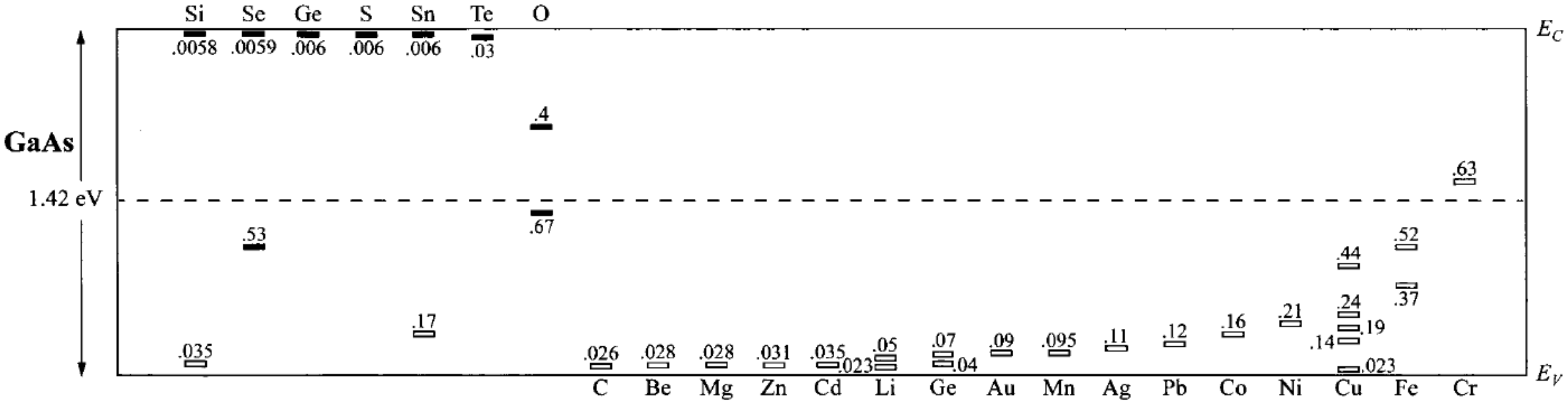
$g_A=4$

At room temperature: $N_D^+ \approx N_D$ $N_A^- \approx N_A$

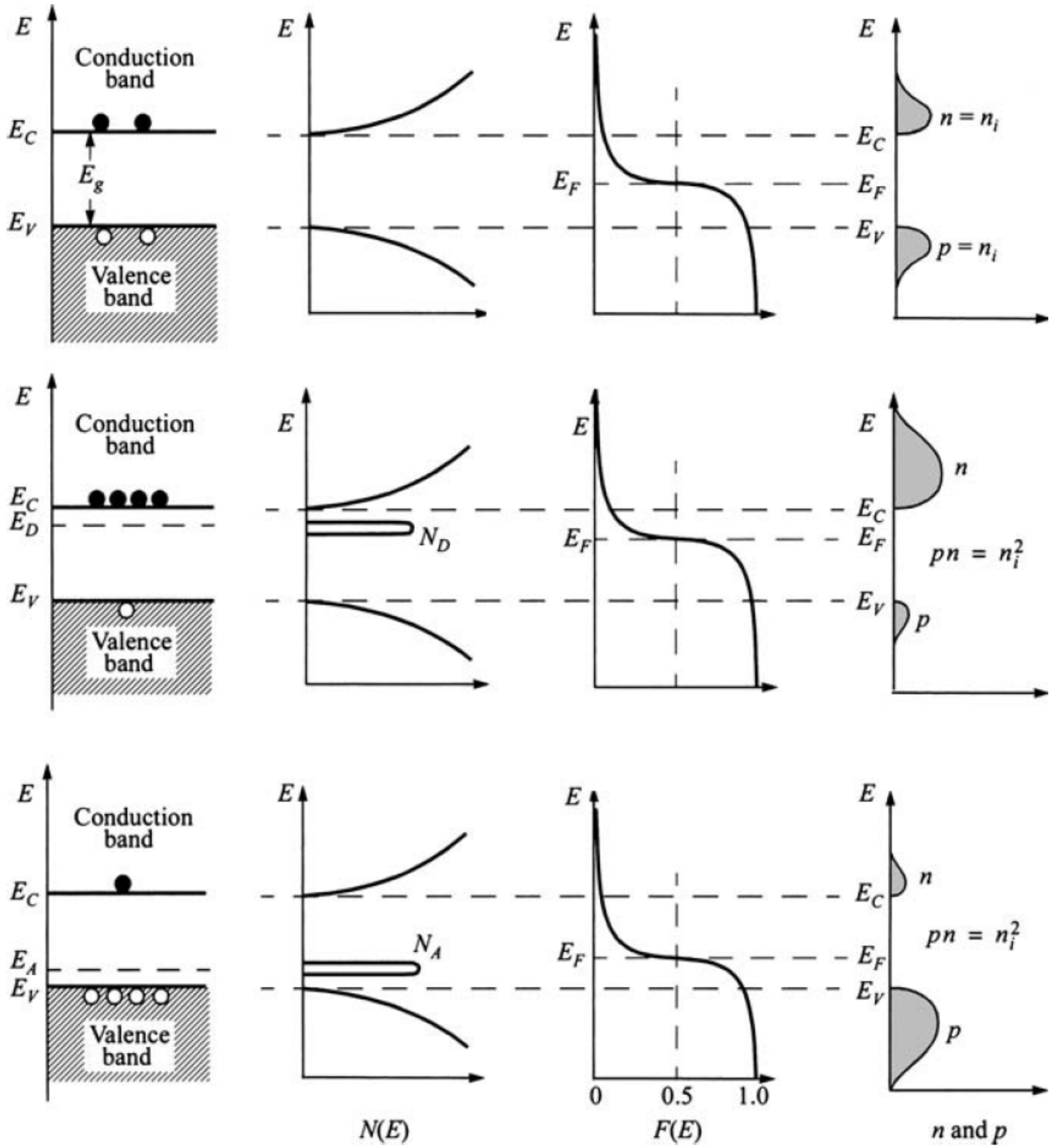
Donor and Accepter levels



(a)



(b)

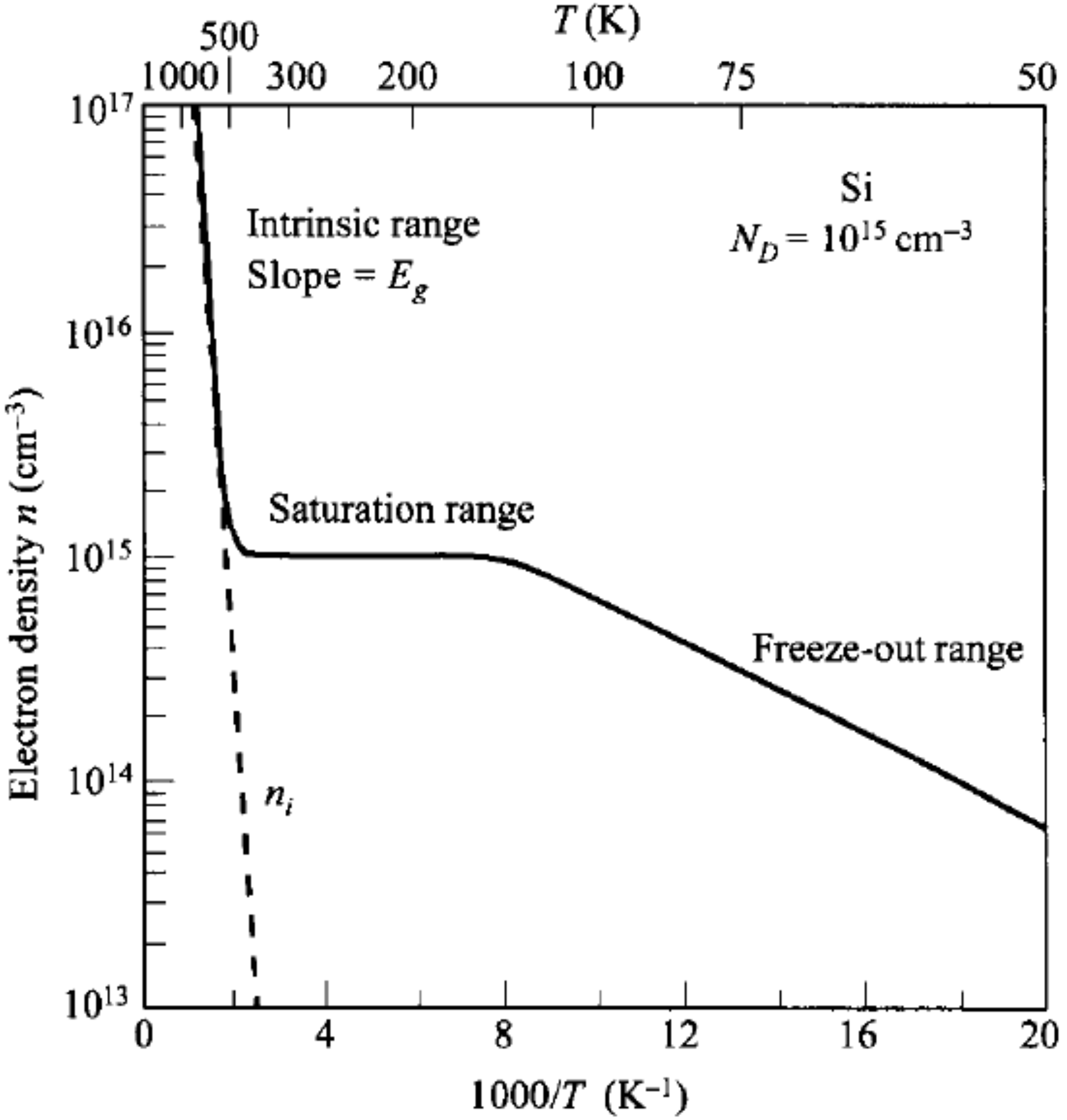


intrinsic

n-material

p-material

Concentration as a function of Temperature



Calculation of Fermi Energy E_F

Neutrality condition: $n + N_A^- = p + N_D^+$

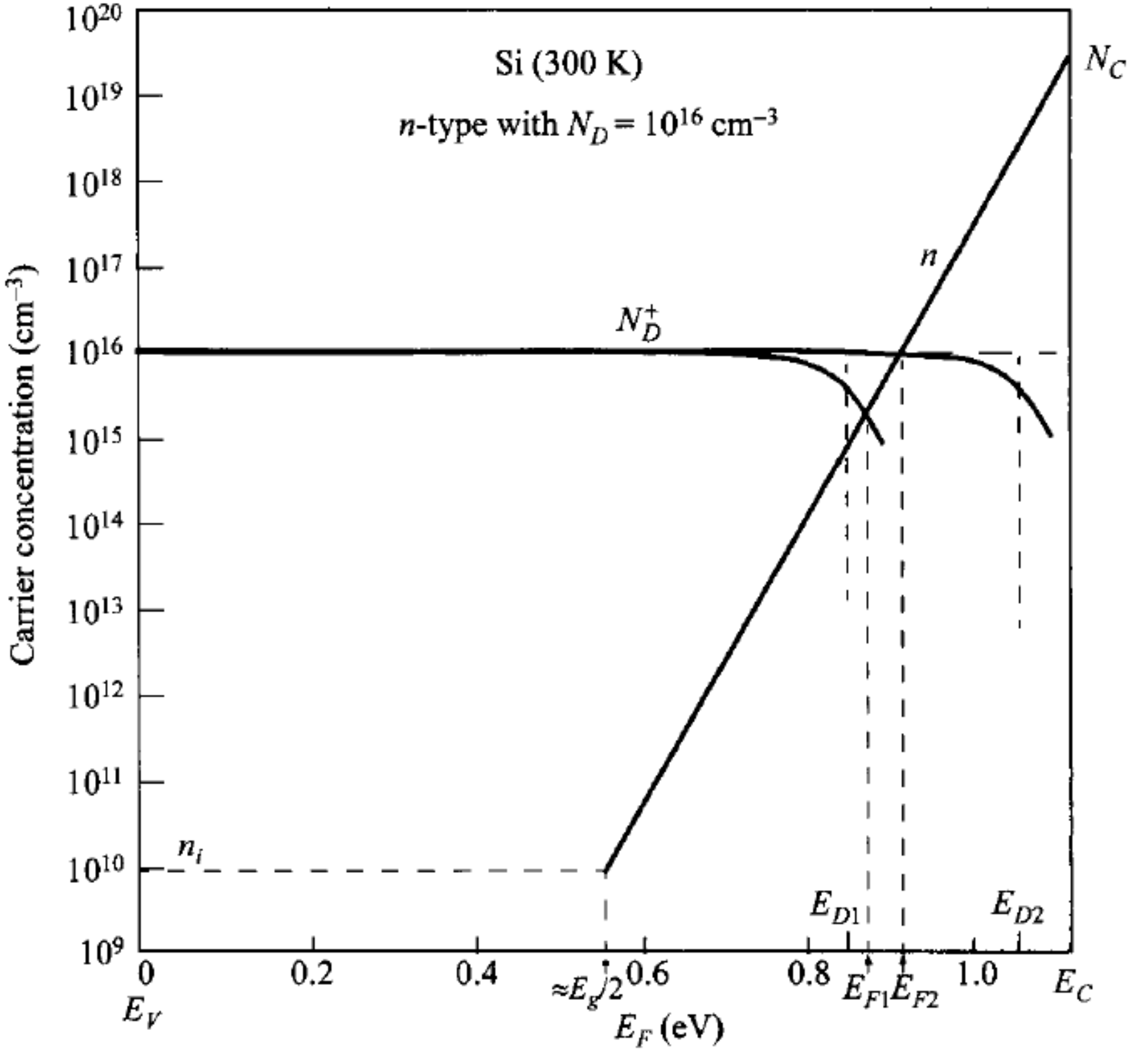
and mass action law still applies: $pn = n_i^2$

consider n-doped: $$\begin{aligned} n &= N_D^+ + p \\ &\approx N_D^+ \end{aligned}$$

$$N_C \exp\left(-\frac{E_C - E_F}{kT}\right) \approx \frac{N_D}{1 + 2\exp[(E_F - E_D)/kT]}$$

E_F can be determined implicitly and then n can be calculated

Calculation of E_F for doped material



Calculation of majority and minority concentrations

$$
\begin{aligned}
n_{no} &= \frac{1}{2}\left[(N_D - N_A) + \sqrt{(N_D - N_A)^2 + 4n_i^2}\right] \\
&\approx N_D \qquad\qquad \text{if} \quad |N_D - N_A| \gg n_i \quad \text{or} \quad N_D \gg N_A .
\end{aligned}
$$

$$p_{no} = \frac{n_i^2}{n_{no}} \approx \frac{n_i^2}{N_D} .$$

Example: $N_D=10^{16}cm^{-3}$ $\Rightarrow$ $n \approx N_D=10^{16}cm^{-3}$

($N_A=0$) => $p \approx n_i^2/N_D=10^{20}/10^{16}=10^4$cm-3

Fermi level determination

$$n_{no} = N_D = N_C \exp\left(-\frac{E_C - E_F}{kT}\right) = n_i \exp\left(\frac{E_F - E_i}{kT}\right)$$

$$E_F - E_i = kT \cdot \ln\left(\frac{N_D}{n_i}\right)$$

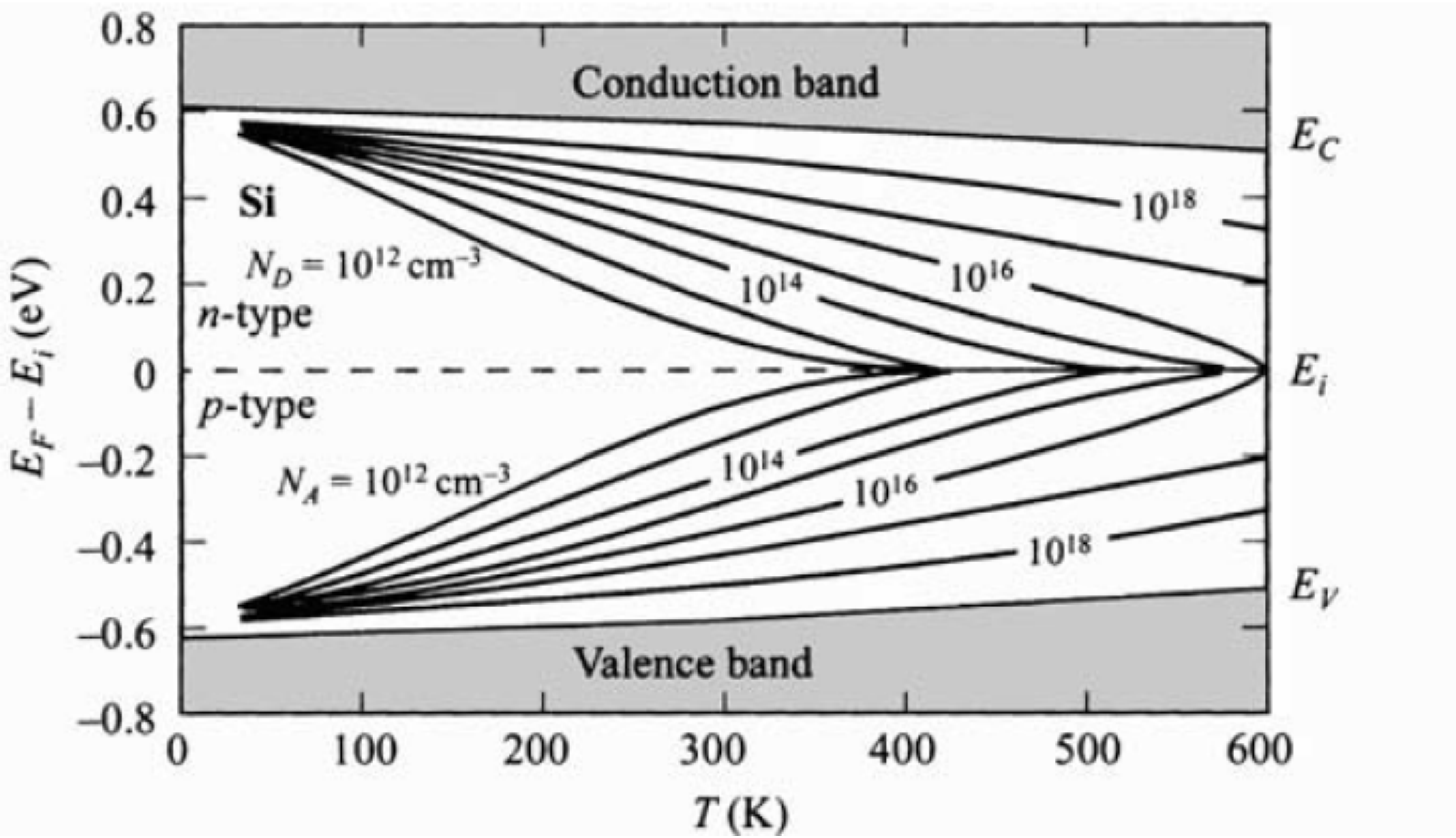
Example:

$N_D=10^{18}cm^{-3}$ gives 18.4kT=0.46eV above $E_g/2$ or

0.1eV below the Valence band edge E_V

Formulaes only valid for non-degenerate case $N_D<N_V$

Position of Fermi level as a function of dopant concentration



Majority and minority concentration for p-type material

$$p_{po} = \frac{1}{2}[(N_A - N_D) + \sqrt{(N_A - N_D)^2 + 4n_i^2}]$$

$$\approx N_A \qquad \text{if} \quad |N_A - N_D| \gg n_i \quad \text{or} \quad N_A \gg N_D$$

$$n_{po} = \frac{n_i^2}{p_{po}} \approx \frac{n_i^2}{N_A},$$

$$p_{po} = N_A = N_V \exp\left(-\frac{E_F - E_V}{kT}\right) = n_i \exp\left(\frac{E_i - E_F}{kT}\right)$$

$$E_i - E_F = kT \cdot \ln\left(\frac{N_A}{n_i}\right)$$

Drift velocity and Mobility

Charge carriers are scattered by phonons or charged impurities, which limits their drift velocity and yields mean free path or mean free time

At low fields, the drift velocity is proportional to the electrical field:

$$\nu_d = \mu \mathscr{E}$$

μ Is the Mobility in cm^2/Vs

Mobility

The mobility due to acoustic phonon scattering is given by:

$$\mu_l = \frac{\sqrt{8\pi}\, q\hbar^4 C_l}{3E_{ds}^2 m_c^{*5/2}(kT)^{3/2}} \propto \frac{1}{m_c^{*5/2} T^{3/2}}$$

C_l is the longitudinal elastic constant
and E_{ds} is the band edge shift per unit dilation

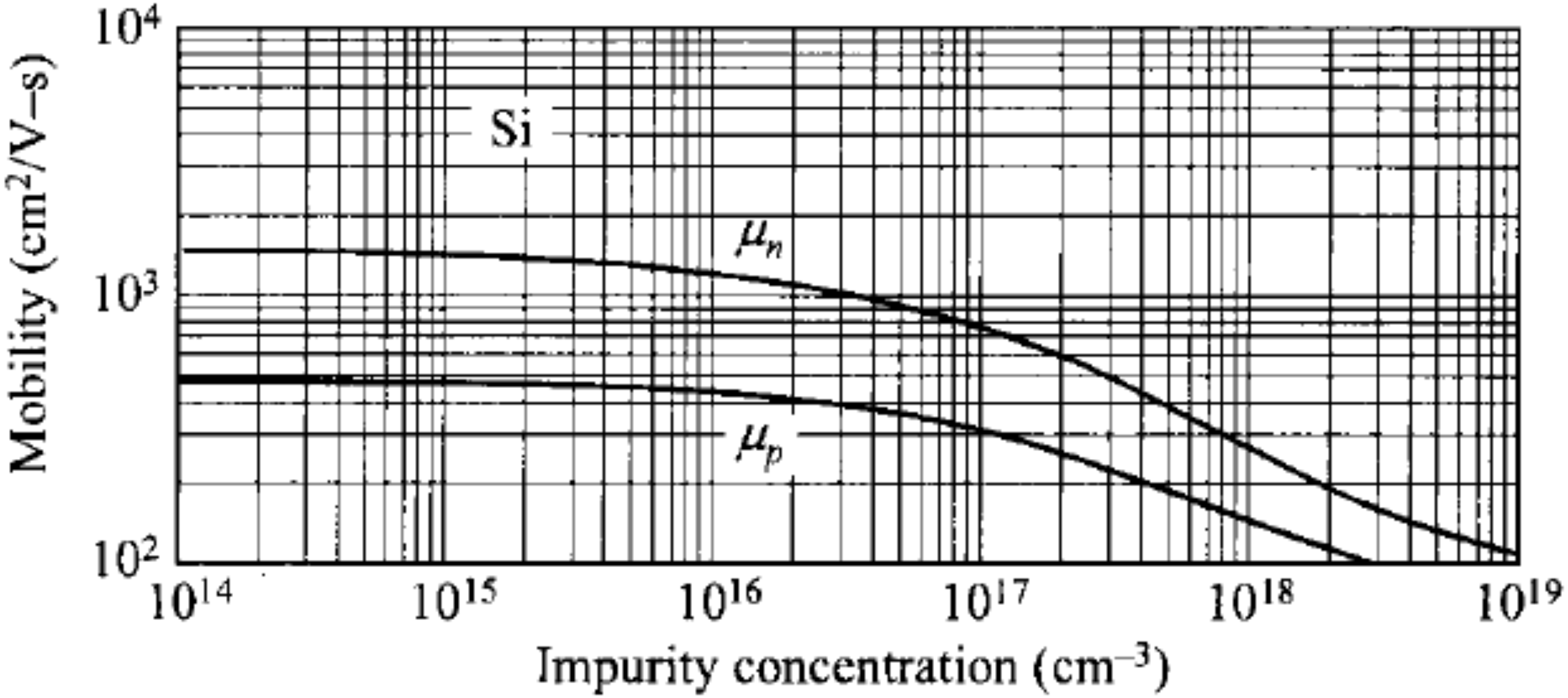
The mobility due to impurity scattering:

$$\mu_i = \frac{64\sqrt{\pi}\, \varepsilon_s^2 (2kT)^{3/2}}{N_I q^3 m^{*1/2}} \left\{ \ln\left[1 + \left(\frac{12\pi\varepsilon_s kT}{q^2 N_I^{1/3}}\right)^2\right]\right\}^{-1} \propto \frac{T^{3/2}}{N_I m^{*1/2}}$$

Mobilities can be combined with the Mathiessen rule:

$$\mu = \left(\frac{1}{\mu_l} + \frac{1}{\mu_i}\right)^{-1}$$

Mobility as a function of dopant concentration



Mean free path λ_m and mean free time τ_m

$$\mu = \frac{q\tau_m}{m^*} = \frac{q\lambda_m}{\sqrt{3kTm^*}}$$

$$\lambda_m = \upsilon_{th}\tau_m \qquad \upsilon_{th} = \sqrt{\frac{3kT}{m^*}}.$$

Thermal velocity

Resistivity ρ and conductivity σ

In semiconductors, both electrons and holes, can contribute to the current density:

$$\begin{aligned} J &= \sigma \mathscr{E} \\ &= q(\mu_n n + \mu_p p)\mathscr{E} \end{aligned}$$

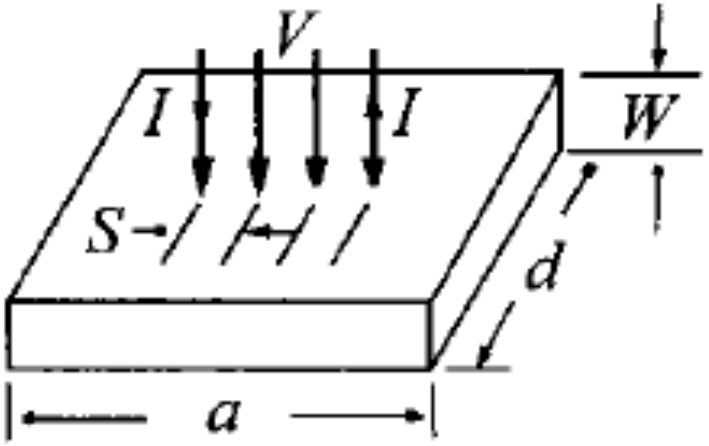
Accordingly, the conductance and resistivity are given:

$$\sigma = \frac{1}{\rho} = q(\mu_n n + \mu_p p)$$

For n-doped material (n>>p):

$$\rho = \frac{1}{q\mu_n n} \qquad \sigma = q\mu_n n$$

Four point probe

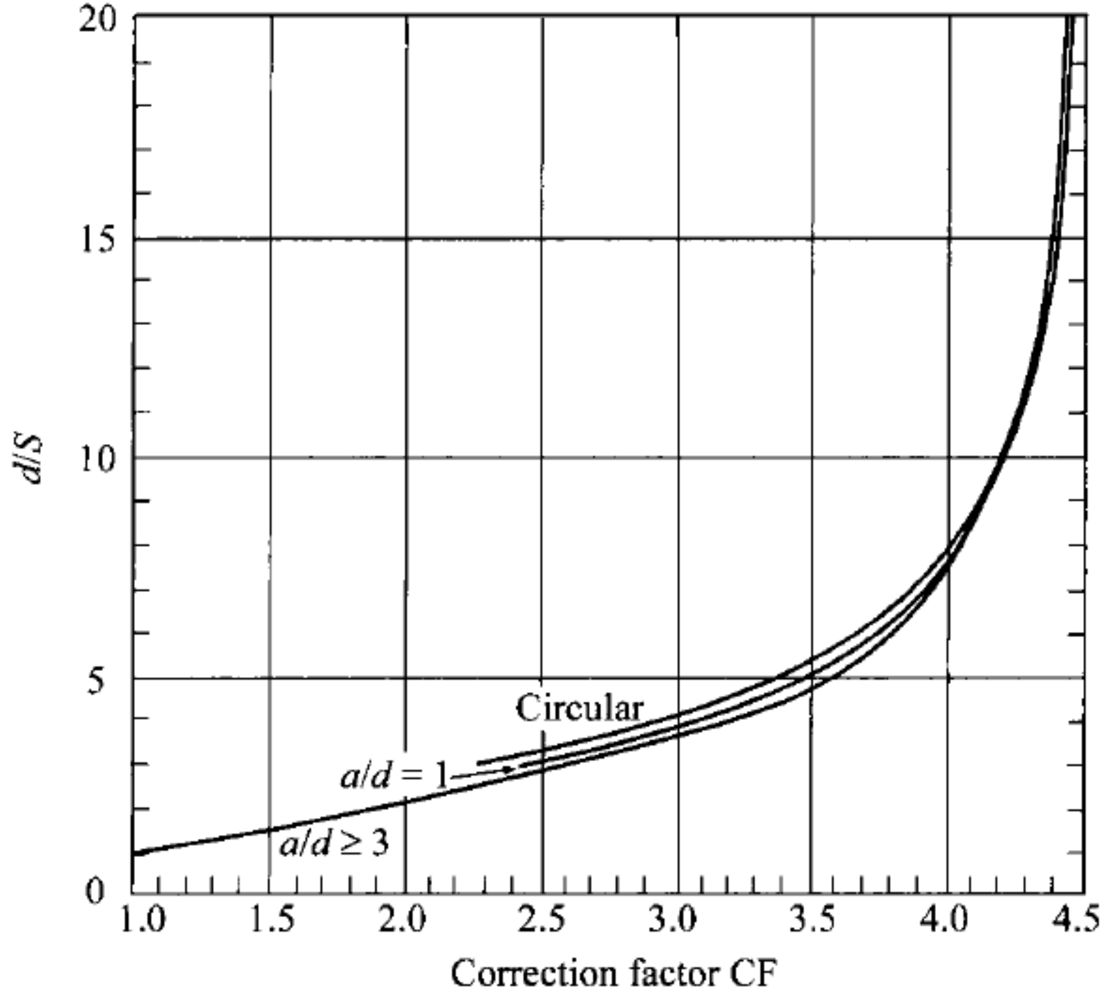


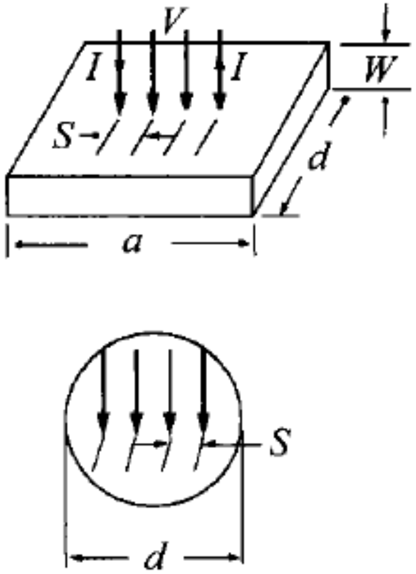
Sheet resistance: $R_\square = \frac{V}{I} \cdot \mathrm{CF} \qquad \Omega/\square$

Correction factor CF=π /ln2=4.54 for d>>S

=> Resistivity is given by: $\rho = R_\square W \qquad \Omega\text{-cm}$

Correction factors CF

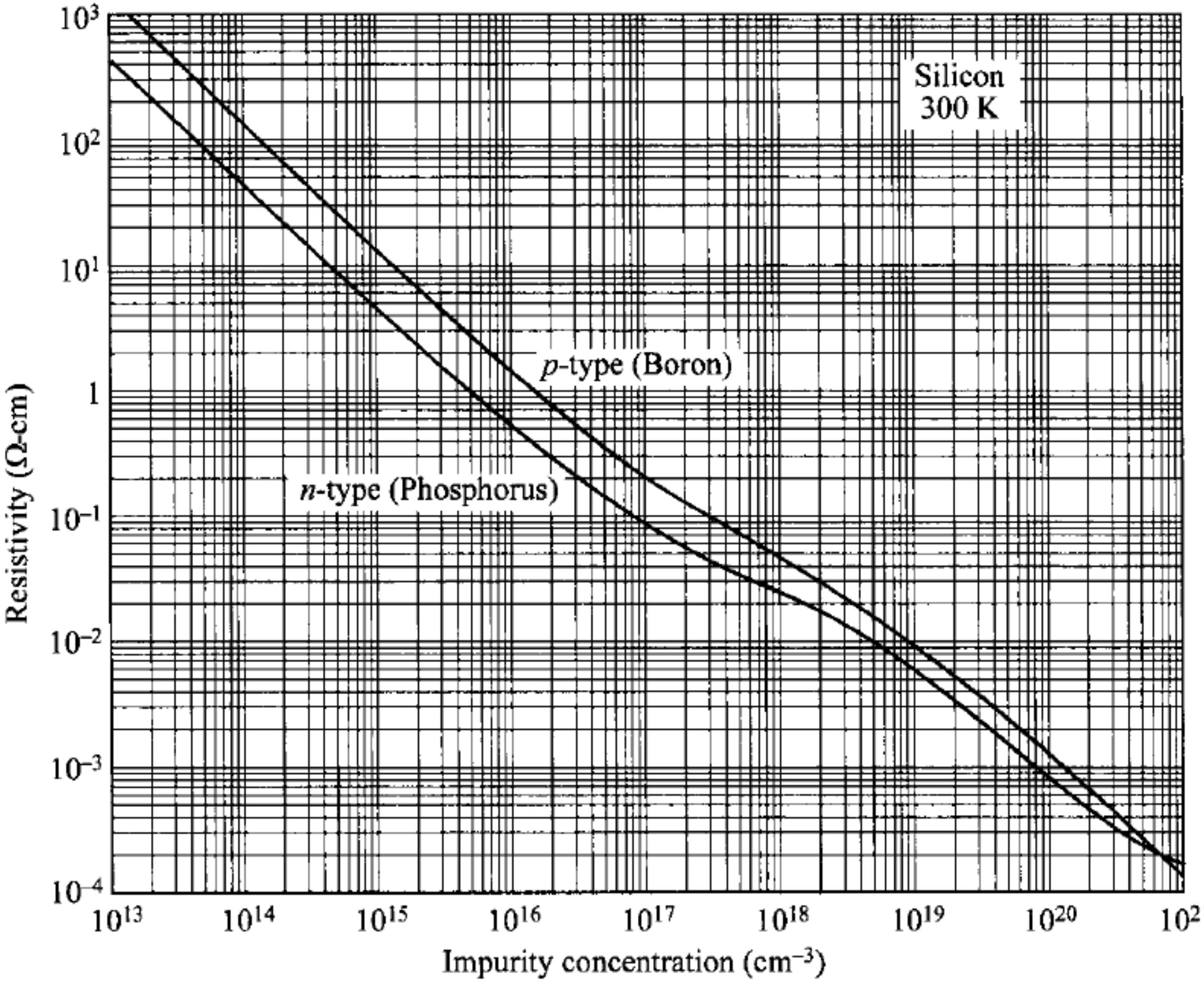




$$R_S = \frac{V}{I}\text{CF} \quad (\Omega/\square)$$

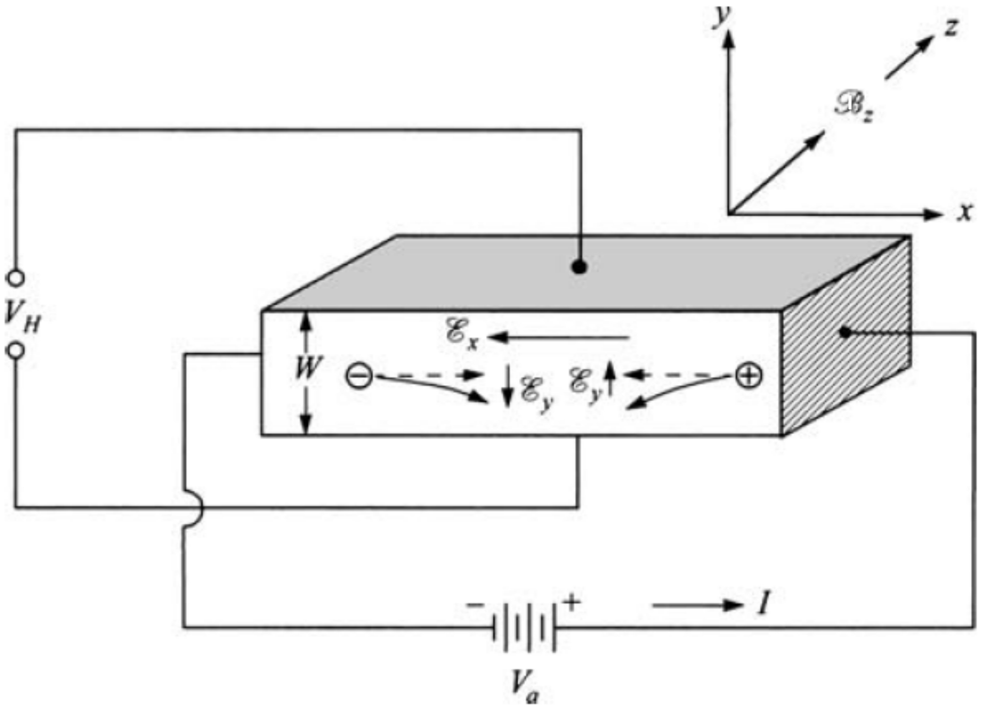
$$\rho = R_S W \quad (\Omega\text{-cm})$$

Example of resistivity ρ vs. impurity concentration N_A or N_D of silicon at 300K



Hall Effect

The hall effect can be used to determine the impurity concentration and the sign of the charge carriers



$$q\mathscr{E}_y = qv_x\mathscr{B}_z$$

$$V_H = \mathscr{E}_y W = \frac{J_x \mathscr{B}_z W}{qp}$$

$$V_H = R_H J_x \mathscr{B}_z W$$

$$R_H = \frac{r_H}{qp} \qquad p \gg n$$

$$R_H = -\frac{r_H}{qn} \qquad n \gg p$$

r_H=1-2 depending on scattering mechanism

High field effects

At thermal equilibrium phonons are emitted and absorbed at equal rate
⇒ Maxwell energy distributions of electrons

At higher fields, electrons acquire more energy and they acquire an average Temperatur Te which is higher than the lattice temperature

Balance of gain of energy from the field and loss of energy through acoustic phonon scattering gives:

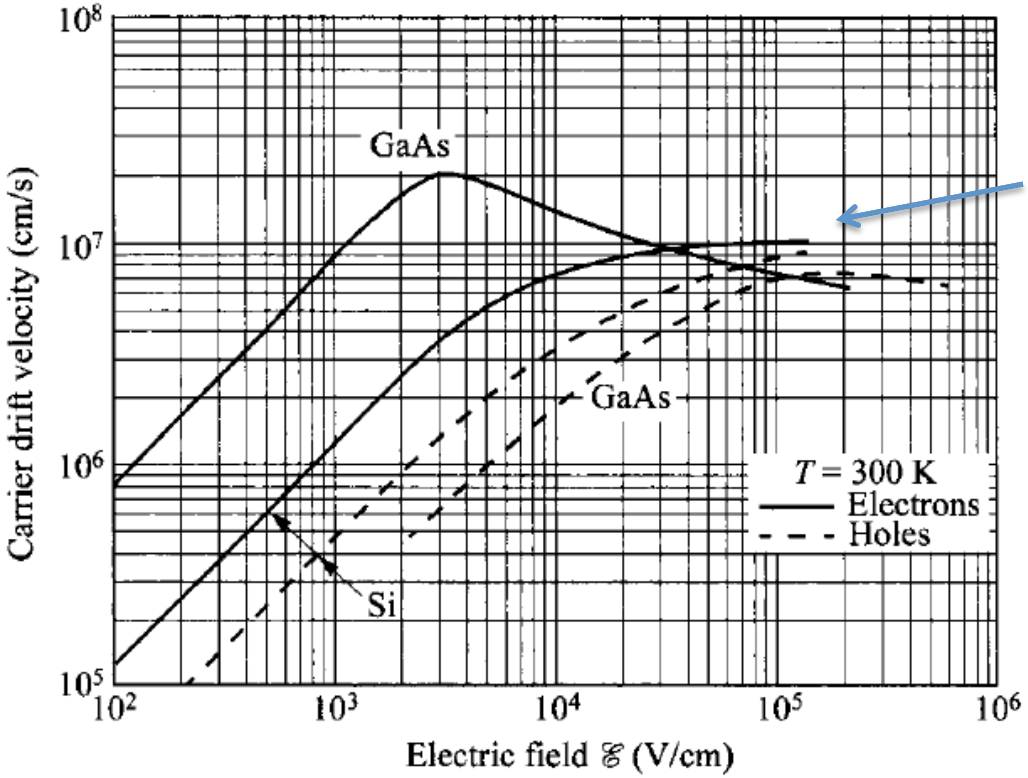
$$v_d = \mu_0 \mathscr{E} \sqrt{\frac{T}{T_e}} \qquad \frac{T_e}{T} = \frac{1}{2}\left[1 + \sqrt{1 + \frac{3\pi}{8}\left(\frac{\mu_0 \mathscr{E}}{c_s}\right)^2}\right]$$

c_s: sound velocity

For high fields, electrons start to interact with optical phonons and v_d saturates

$$v_s = \sqrt{\frac{8E_p}{3\pi m_0}} \approx 10^7 \text{ cm/s}$$

Drift velocity as a function of Field



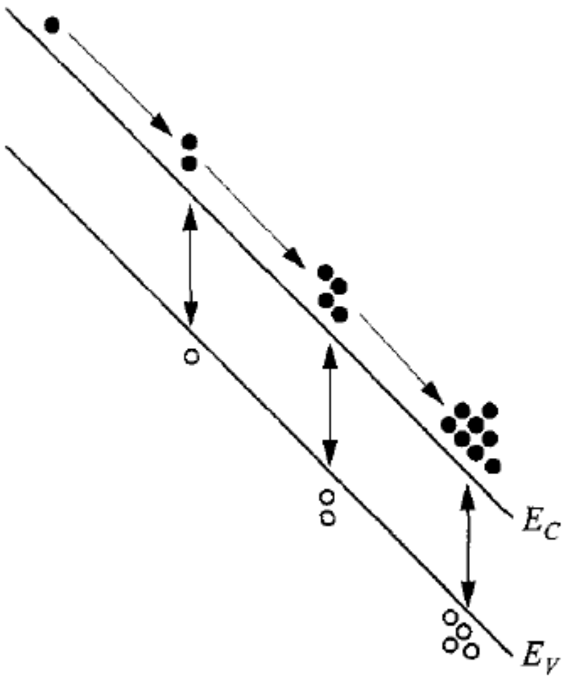
Saturation due to scattering with optical phonons

Empirical formula:

$$v_d = \frac{\mu_0 \mathscr{E}}{\left[1 + (\mu_0 \mathscr{E}/v_s)^{C_2}\right]^{1/C_2}}$$

$C_2 \approx 2$ for electrons
$C_2 \approx 1$ for holes

Impact Ionization



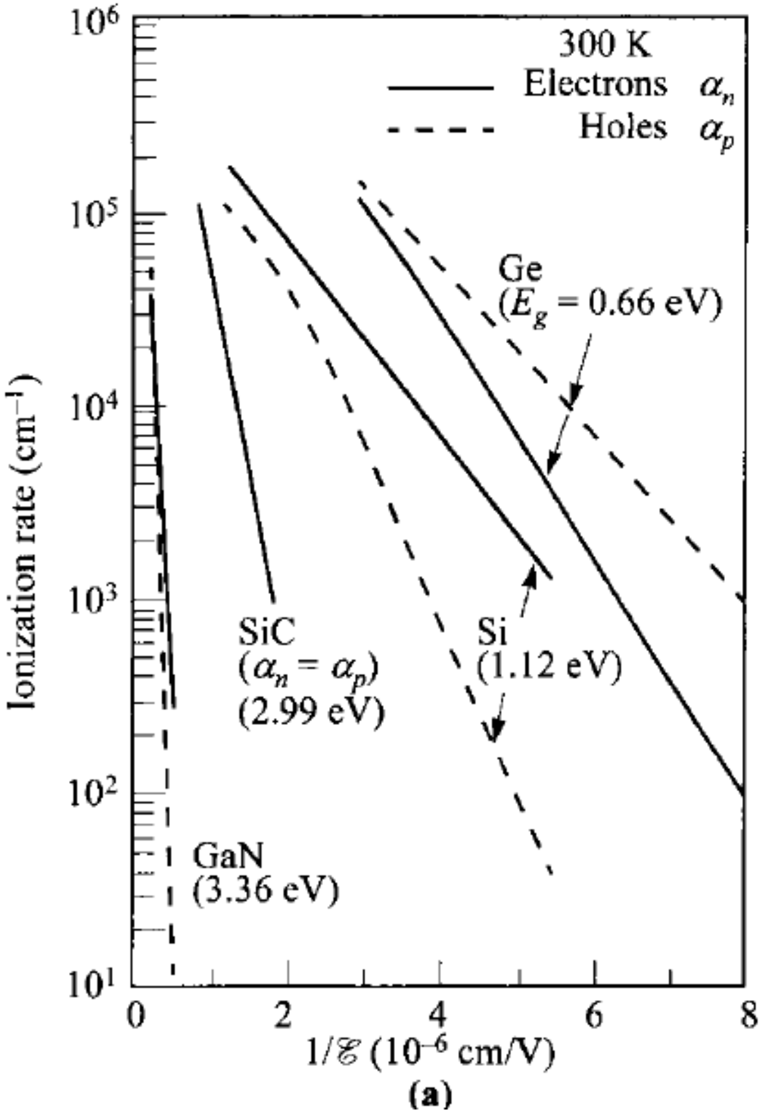
At high fields charge carriers can start
Create electron hole pairs, called
Impact ionization

Si: E_I=3.6eV for electrons and E_I=5eV for holes

$$\alpha(\mathscr{E}) = \frac{q\mathscr{E}}{E_I}\exp\left(-\frac{\mathscr{E}_I}{\mathscr{E}}\right)$$

Impact ionization rate

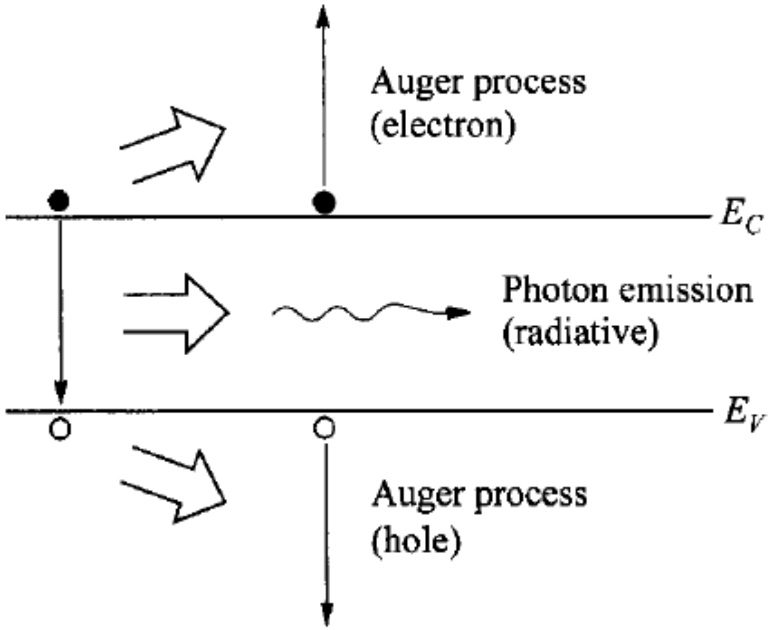
Ionization rate for different materials



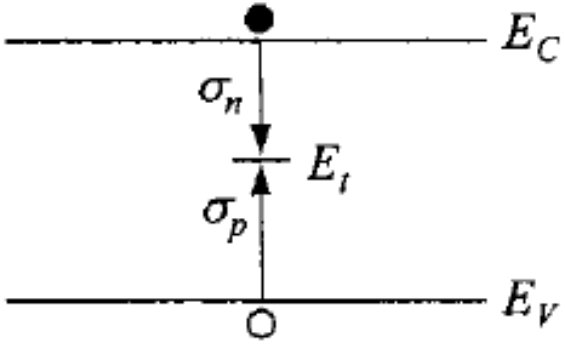
Note:
Ionization rate decreases with larger band gap.
For this reason materials with larger band gap have higher breakdown voltage.

Recombination, Generation and Carrier life time

If thermal equilibrium ($pn=n_i^2$) is disturbed there will be either recombination processes $pn>n_i^2$) or generation processes($pn<n_i^2$) to recover equilibrium



Recombination processes:
Band to band recombination of electron and
hole and creation of photons or Auger electrons



non-radiative process
through gap state

Recombination rates

Band to band recombination (most common for direct sc)

$$R_e = R_{ec} p n$$

$R_{ec} \approx 10^{-10} cm^3 s^{-1}$ for direct semiconductor like GaAs

$R_{ec} \approx 10^{-15} cm^3 s^{-1}$ for indirect semiconductor like Si

Generation rate is related to recombination rate: $R_{ec} = \frac{G_{th}}{n_i^2}$

In thermal equilibrium: $R_e = G_{th}$

Low level injection or illumination

An excess carrier density $\Delta n=\Delta p$ is created by low level injection or illiumination

For n-type material:

$$p_n=p_{n0}+\Delta p$$

$$n_n \approx N_D$$

Net transition rate:

$$U = R_e - G_{th} = R_{ec}(pn - n_i^2)$$
$$\approx R_{ec}\Delta p N_D \equiv \frac{\Delta p}{\tau_p}$$

Life time for holes in n-material:

$$\tau_p = \frac{1}{R_{ec}N_D}$$

Similarly for p-material:

$$\tau_n = \frac{1}{R_{ec}N_A}$$

Shockley-Read-Hall statistics

For indirect semiconductors like Si or Ge, the dominant recombination process is electron hole recombination via interface trap states E_T

Net transition rate is given by:

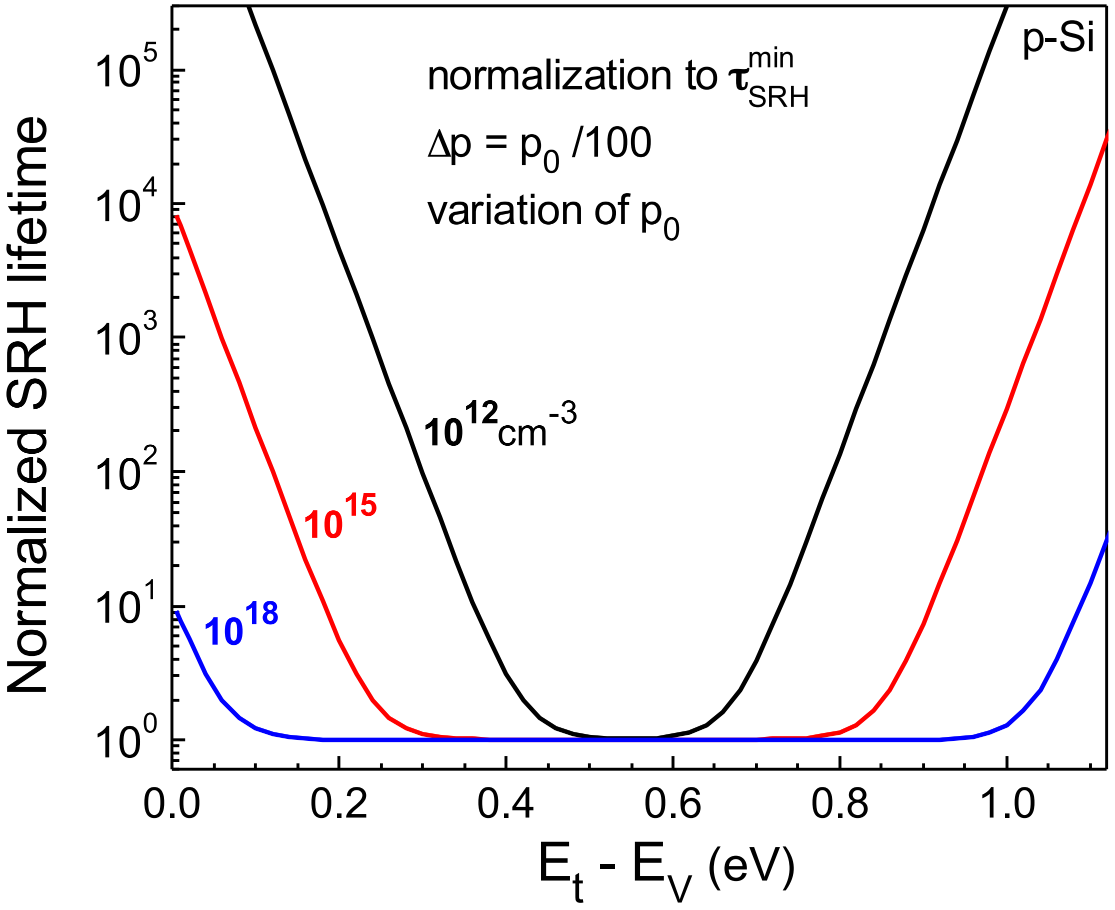
$$U = \frac{\sigma_n \sigma_p v_{th} N_t (pn - n_i^2)}{\sigma_n\left[n + n_i \exp\left(\frac{E_t - E_i}{kT}\right)\right] + \sigma_p\left[p + n_i \exp\left(\frac{E_i - E_t}{kT}\right)\right]}$$

Most dominant are trap states close to mid gap E_i

Then for n-type material: $\tau_p = \frac{1}{\sigma_p v_{th} N_t}$ p-type material: $\tau_n = \frac{1}{\sigma_n v_{th} N_t}$

Example: Au in Si reduces lifetime 2 10^{-6}s to 2 10^{-9}s with concentration from 10^{14} to 10^{17}cm-3

SRH lifetimes as a function of E_t



Example for minimum life time due to SRH mechanism

$$\tau_{h,SRH}^{\min} = 1 / N_t \sigma_{e(h)} \mathrm{v}_{th} = 10^{-4}\ \mathrm{sec}$$

where $N_t = 10^{12}\mathrm{cm}^{-3}$ $\sigma = 10^{-15}\mathrm{cm}^2$ $\mathrm{v} = 10^5\mathrm{m/s}$

Thus, in solar cells low trap densities of $10^{12}\mathrm{cm}^{-3}$ have to reached to meet the required life times of $100\mu\mathrm{s}$

Diffusion


Diffusion

Whenever locally higher concentrations occur diffusion of the charge carriers will lead to a transport from regions of high concentration to low concentrations:

$$\left.\frac{d\Delta n}{dt}\right|_x = -D_n \frac{d\Delta n}{dx}$$

Which leads to diffusion currents:

$$J_n = qD_n \frac{d\Delta n}{dx}$$

$$J_p = -qD_p \frac{d\Delta p}{dx}$$

Diffusion coefficients are related to the mobilities by the Einstein relations:

$$D_n = \left(\frac{kT}{q}\right)\mu_n$$

$$D_p = \left(\frac{kT}{q}\right)\mu_p$$

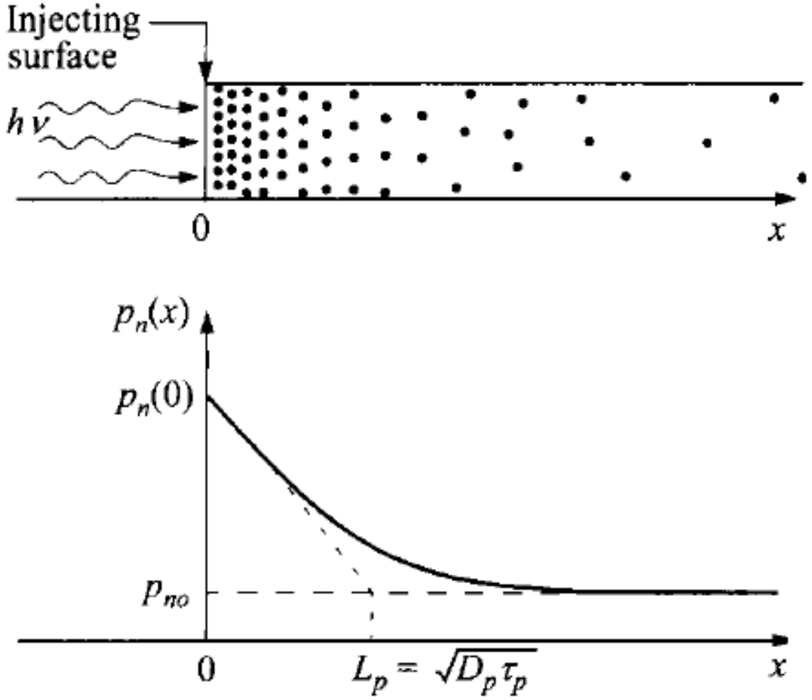
Diffusion length

$$L_d = \sqrt{D\tau}$$

Distance , which carriers can travel before they are annihilated
τ carrier life time

Example:
Si at 300K: D=36cm^2/s
τ =10^{-4}sec
L$_d$=1.5 10^{-2}cm=147μm

Decay of excess carriers with distance



$$L_p = (D_p \tau_p)^{1/2}$$

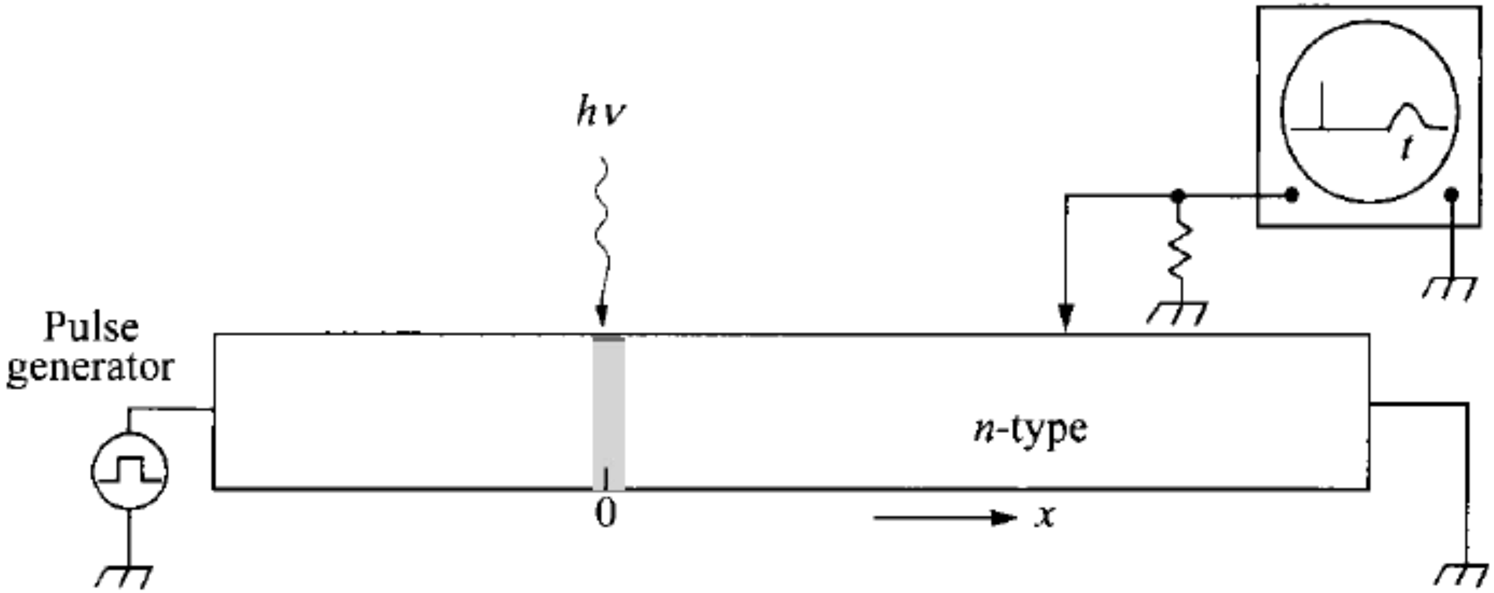
Maximum of diffusion length
for Si: cm
GaAs: 10^{-2}cm

Inject carriers by photo irradiation (e.g. UV-light).
Carrier density decays exponentially with distance from the surface

$$\frac{\partial p_n}{\partial t} = 0 = -\frac{p_n - p_{no}}{\tau_p} + D_p \frac{\partial^2 p_n}{\partial x^2}$$

$$p_n(x) = p_{no} + [p_n(0) - p_{no}] \exp\left(-\frac{x}{L_p}\right)$$

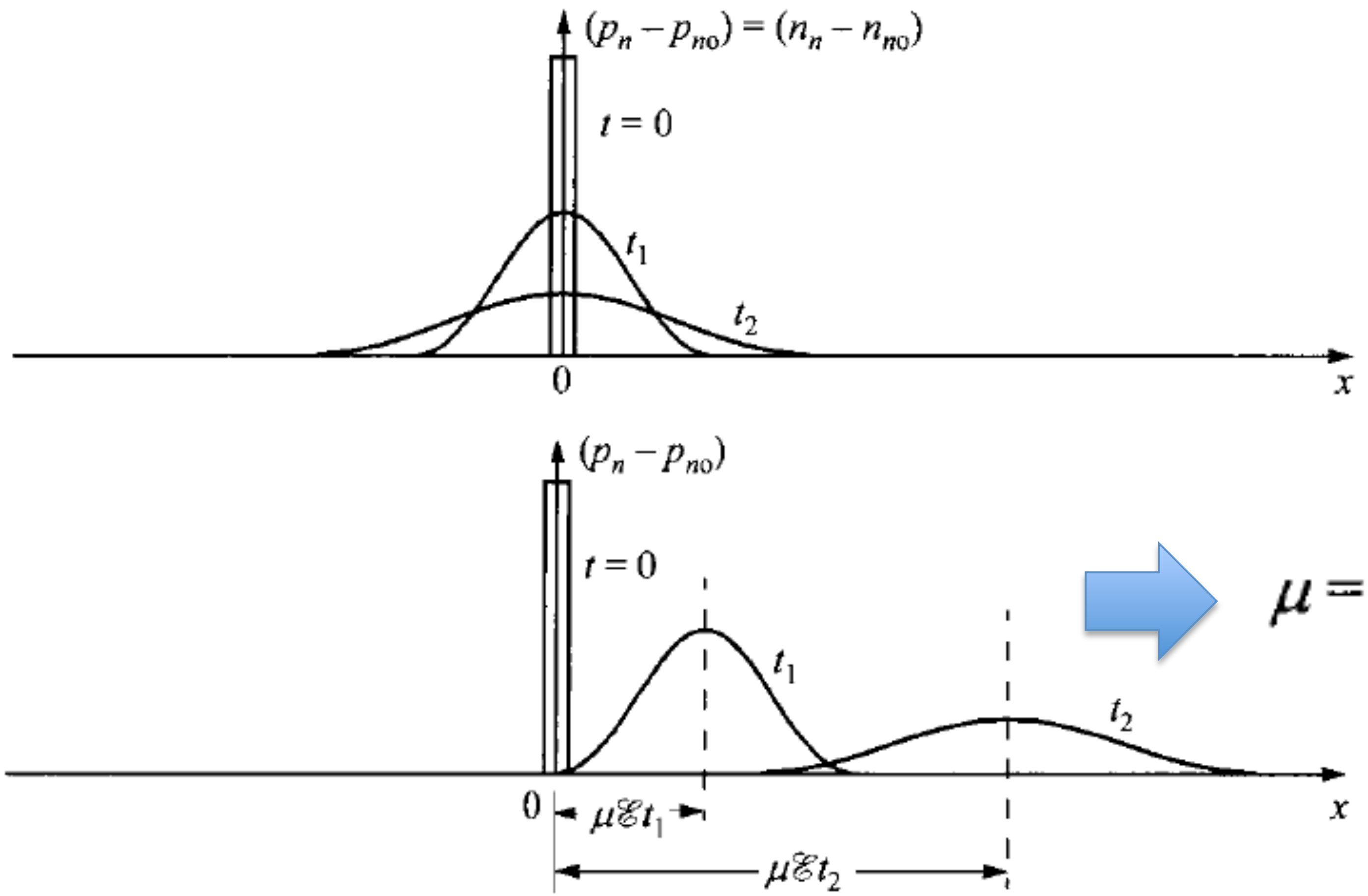
Decay of excess carriers in time and distance



$$\frac{\partial p_n}{\partial t} = -\frac{p_n - p_{no}}{\tau_p} + D_p \frac{\partial^2 p_n}{\partial x^2}$$

$$p_n(x,t) = \frac{N'}{\sqrt{4\pi D_p t}} \exp\left(-\frac{x^2}{4D_p t} - \frac{t}{\tau_p}\right) + p_{no}$$

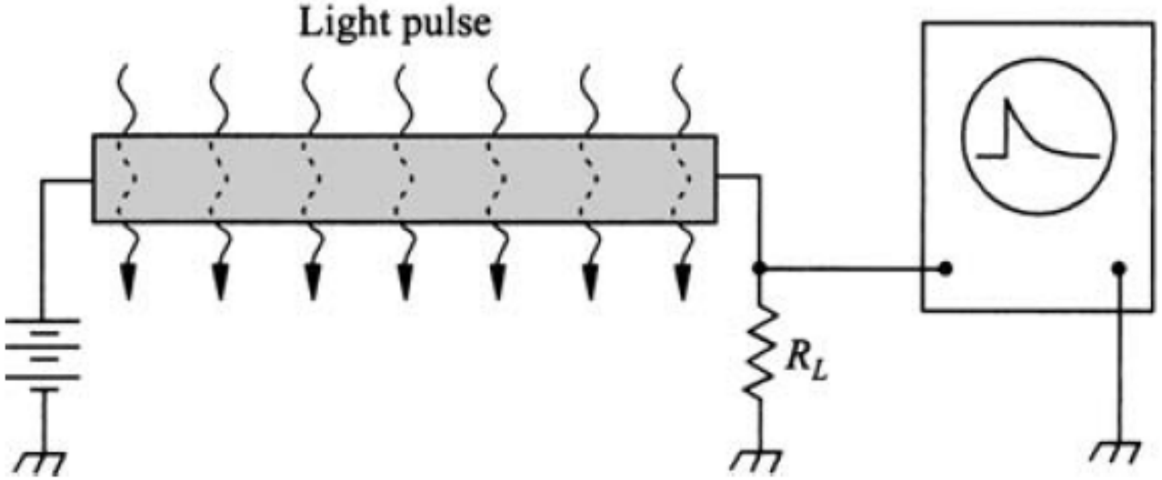
Determine diffusion coefficient and drift mobility

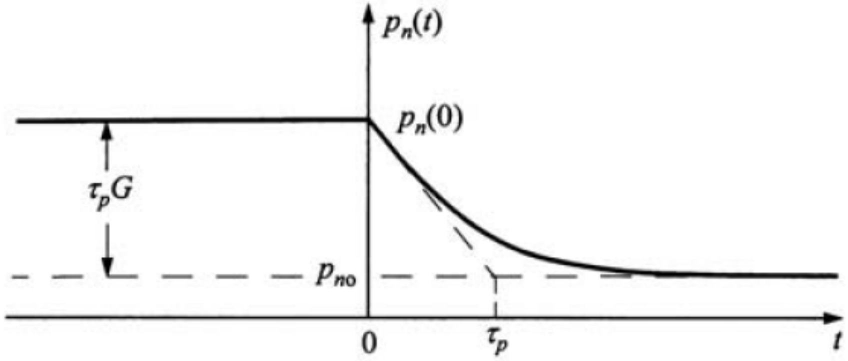


$$\mu = x/\mathscr{E}t$$

Haynes-Shockley experiment

Determine minority carrier life time $\tau_p(_n)$





After light is switched off:

$$\frac{dp_n}{dt} = -\frac{p_n - p_{no}}{\tau_p}$$

$$p_n(t) = p_{no} + \tau_p G_p \exp\left(-\frac{t}{\tau_p}\right)$$