“Complementi di Fisica”
Lecture 3

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Course Outline - Reminder

- The physics of semiconductor devices: an introduction
  - Basic properties; energy bands, density of states
  - Equilibrium carrier concentration (“intrinsic”, “extrinsic”)
  - Carrier transport phenomena
    - Drift and Diffusion
    - Generation and Recombination
    - Continuity equations
- Quantum Mechanics: an introduction
- Advanced semiconductor fundamentals

- Lecture 2: intrinsic carrier concentrations…

Outline – Lecture 3

- “Intrinsic” (= pure) semiconductor *at equilibrium*
  - Equilibrium: computation of “carriers concentration”:

    Concentration (carriers per unit volume) =

    = sum (integral) over energy of:

      (Available energy levels, per unit volume and per energy interval)

      × (probability of filling the levels, per energy interval)

- “Extrinsic” (= doped) semiconductor *at equilibrium*
  - “donors” and “acceptors”: bond model
  - “donors” and “acceptors”: energy band model:
    - band diagrams
    - density of states
    - carriers concentration,
    - Fermi level

Intrinsic semiconductors

Fermi-Dirac distribution function

Intrinsic carriers concentration, Fermi level

Fermi probability distribution function

- Electrons fill up available states following the Pauli principle (two electrons with opposite spin for each level)
- Probability distribution function (Fermi-Dirac, more details in the second part of the course):

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

$$E=E_F \Rightarrow F(E)=1/2$$

$$E\rightarrow\infty \Rightarrow F(E)\rightarrow 0$$

$$E\rightarrow-\infty \Rightarrow F(E)\rightarrow 1$$

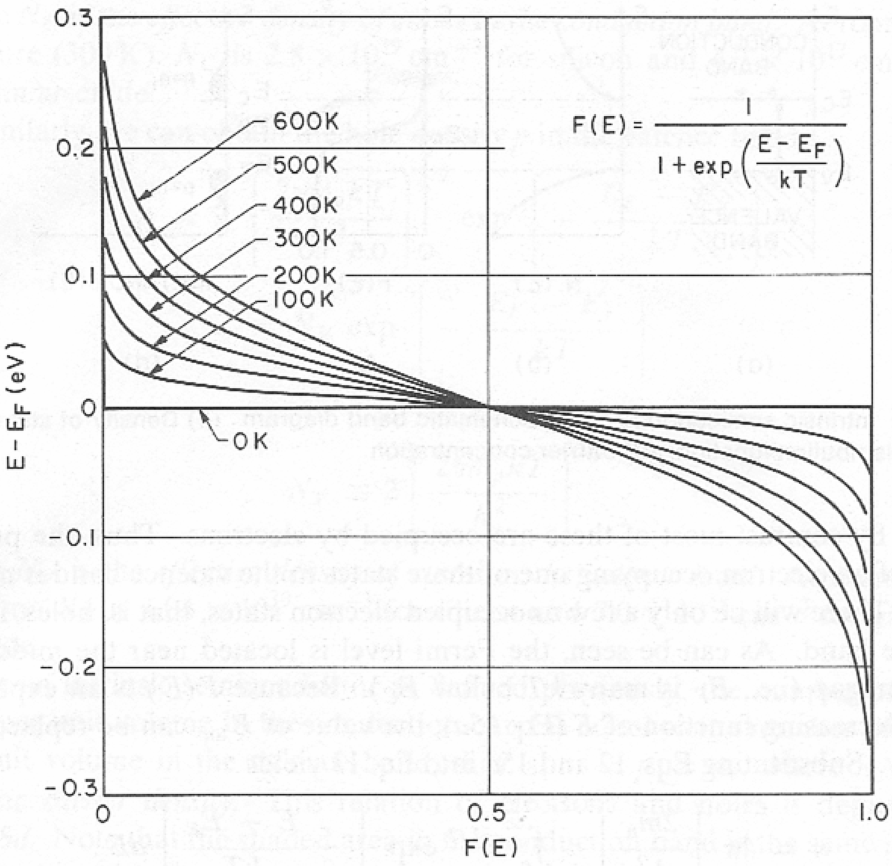
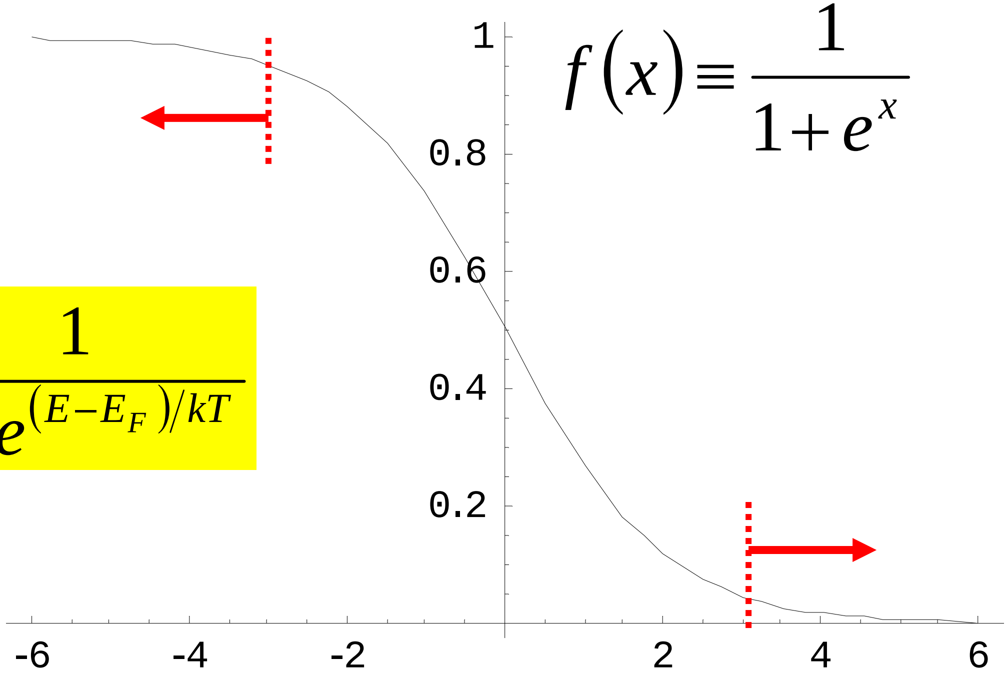


Fig. 14 Fermi distribution function $F(E)$ versus $(E - E_F)$ for various temperatures.

$k = 8.617\times10^{-5}\ eV/K$ Boltzmann constant, T temperature (K)

Fermi pdf: approximate expressions

- Fermi pdf



$$f(x) \equiv \frac{1}{1+e^{x}}$$

$$F(E) \equiv \frac{1}{1+e^{(E-E_F)/kT}}$$

$$x = \frac{E-E_F}{kT}$$

- approximate expressions for energies far enough from E_F:

$$E-E_F > 3kT \Rightarrow F(E) \approx e^{-(E-E_F)/kT} \qquad \left(\boxed{x>3} \;\Rightarrow \frac{1}{1+e^{x}} \approx e^{-x} \right)$$

$$E-E_F < -3kT \Rightarrow F(E) \approx 1-e^{-(E_F-E)/kT} \qquad \left(\boxed{x<-3} \;\Rightarrow \frac{1}{1+e^{x}} \approx 1-e^{x} \right)$$

Fermi pdf: approximate expressions

- Simpler expressions for energies far enough from E_F:

$$F(E) \cong e^{-(E-E_F)/kT} \quad \text{for} \quad E-E_F > 3kT$$

$$F(E) \cong 1-e^{-(E_F-E)/kT} \quad \text{for} \quad E-E_F < -3kT$$

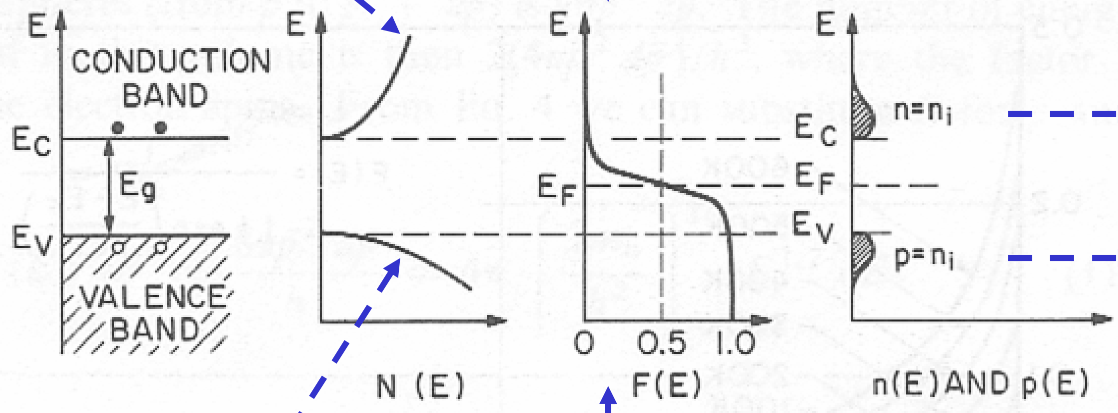
Intrinsic carrier concentrations

$$g_C(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_C)}}{\pi^2 \hbar^3}$$

$$F(E) \cong e^{-(E-E_F)/kT}$$

Effective density of states
In the conduction band

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



$$n \cong N_C e^{-(E_F - E_C)/kT}$$

$$p \cong N_V e^{-(E_V - E_F)/kT}$$

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

$$1 - F(E) \cong e^{-(E_F - E)/kT}$$

$$g_V(E) = \frac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3}$$

Effective density of states
In the valence band

Exercise 2.1 Integrate g(E)F(E) to obtain n and p

Intrinsic electron concentration *n*

- Explicit computation for electrons:

$$n = \int_{E_C}^{\infty} g_C(E) F(E)\, dE =$$

$$= 4\pi \left(\frac{2m_n^*}{h^2}\right)^{3/2} \int_{E_C}^{\infty} (E - E_C)^{1/2} e^{-(E-E_F)/kT}\, dE =$$

$$= 4\pi \left(\frac{2m_n^*}{h^2}\right)^{3/2} \int_{0}^{\infty} E'^{1/2} e^{-(E'+E_C-E_F)/kT}\, dE' =$$

$$= 4\pi \left(\frac{2m_n^*}{h^2}\right)^{3/2} (kT)^{3/2} \exp\left(-\frac{E_C - E_F}{kT}\right) \int_0^{\infty} x^{1/2} e^{-x}\, dx =$$

$$= 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2} \exp\left(-\frac{E_C - E_F}{kT}\right)$$

$g_C(E)$ state density

Fermi f. for $E - E_F > 3kT$

$$F(E) \approx e^{-(E-E_F)/kT}$$

change variables:

$$E' = E - E_C \qquad dE' = dE$$

$$x = \frac{E'}{kT} \qquad dE' = kT\,dx$$

$$\int_0^{\infty} x^{1/2} e^{-x}\, dx = \frac{\sqrt{\pi}}{2}$$

Intrinsic hole concentration *p*

- Explicit computation for holes:

$$p = \int_{-\infty}^{E_V} g_V(E)\left(1 - F(E)\right) dE =$$

$$= 4\pi \left(\frac{2m_p^*}{h^2} \right)^{3/2} \int_{-\infty}^{E_V} \left(E_V - E\right)^{1/2} e^{-(E_F - E)/kT} dE =$$

$$= 4\pi \left(\frac{2m_p^*}{h^2} \right)^{3/2} \int_{0}^{\infty} E'^{1/2} e^{-(E' + E_F - E_V)/kT} dE' =$$

$$= 4\pi \left(\frac{2m_p^*}{h^2} \right)^{3/2} (kT)^{3/2} \exp\left(- \frac{E_F - E_V}{kT} \right) \int_0^\infty x^{1/2} e^{-x} dx =$$

$$= 2 \left(\frac{2\pi m_p^* \enclose{circle}{kT}}{h^2} \right)^{3/2} \exp\left(- \frac{\enclose{circle}{E_F} - E_V}{\enclose{circle}{kT}} \right)$$

$g_V(E)$ state density

$1 - F(E)$ for $E - E_F < -3kT$

$1 - F(E) \approx e^{-(E_F - E)/kT}$

change variables:

$E' = E_V - E \qquad dE' = -dE$

$x = \dfrac{E'}{kT} \qquad dE' = kT\,dx$

$$\int_0^\infty x^{1/2} e^{-x} dx = \frac{\sqrt{\pi}}{2}$$

Intrinsic Fermi level and carrier density

"Effective density of states"
In the conduction band

$$N_C \equiv 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2} \cong 2.8\times10^{19}\,cm^{-3}\ \text{(Si)},$$

$$[T \approx 300K] \qquad \cong 4.7\times10^{17}\,cm^{-3}\ \text{(GaAs)}$$

"Effective density of states"
In the valence band

$$N_V \equiv 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2} \cong 1.04\times10^{19}\,cm^{-3}\ \text{(Si)}$$

$$[T \approx 300K] \qquad \cong 7.0\times10^{18}\,cm^{-3}\ \text{(GaAs)}$$

$$n \cong N_C e^{-(E_F-E_C)/kT}$$

$$p \cong N_V e^{-(E_V-E_F)/kT}$$

For an intrinsic semiconductor:

$$n = p = n_i$$

Intrinsic carrier density

$$n = p \Rightarrow E_i = E_F = \frac{E_C+E_V}{2} + \frac{kT}{2}\ln\left(\frac{N_V}{N_C}\right) = \frac{E_C+E_V}{2} + \frac{3kT}{4}\ln\left(\frac{m_p}{m_n}\right) \Rightarrow \boxed{E_i \cong \frac{E_C+E_V}{2}}$$

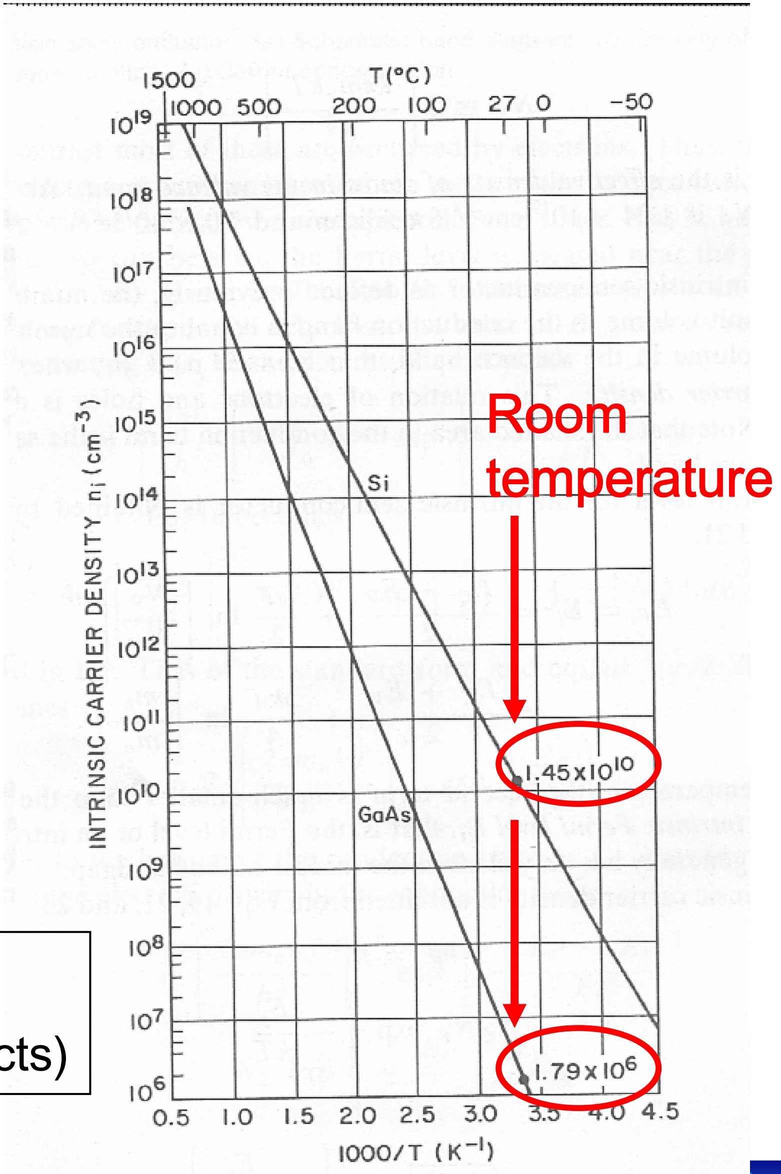
Intrinsic Fermi level

"mass action law": at thermal equilibrium:

$$np = n_i^2 = N_C N_V e^{-E_g/kT} \quad\Rightarrow\quad n_i = \sqrt{N_C N_V}\, e^{-E_g/2kT}$$

Intrinsic carrier densities

- Temperature dependence
  - increase with temperature
  - smaller with larger E_g
- Caveats:
  - Pure Si: very low conductivity: $\sigma \approx 10^{-6} (\Omega\ \mathrm{cm})^{-1}$ at $T \approx 300\mathrm{K}$
  - However, in practice dominated by defects (Kowalski method: typically $10^{11}/\mathrm{cm}^2$) $\Rightarrow \sigma \approx 10^{-5} (\Omega\ \mathrm{cm})^{-1}$
  - Doping is needed in practice, to control conductivity!

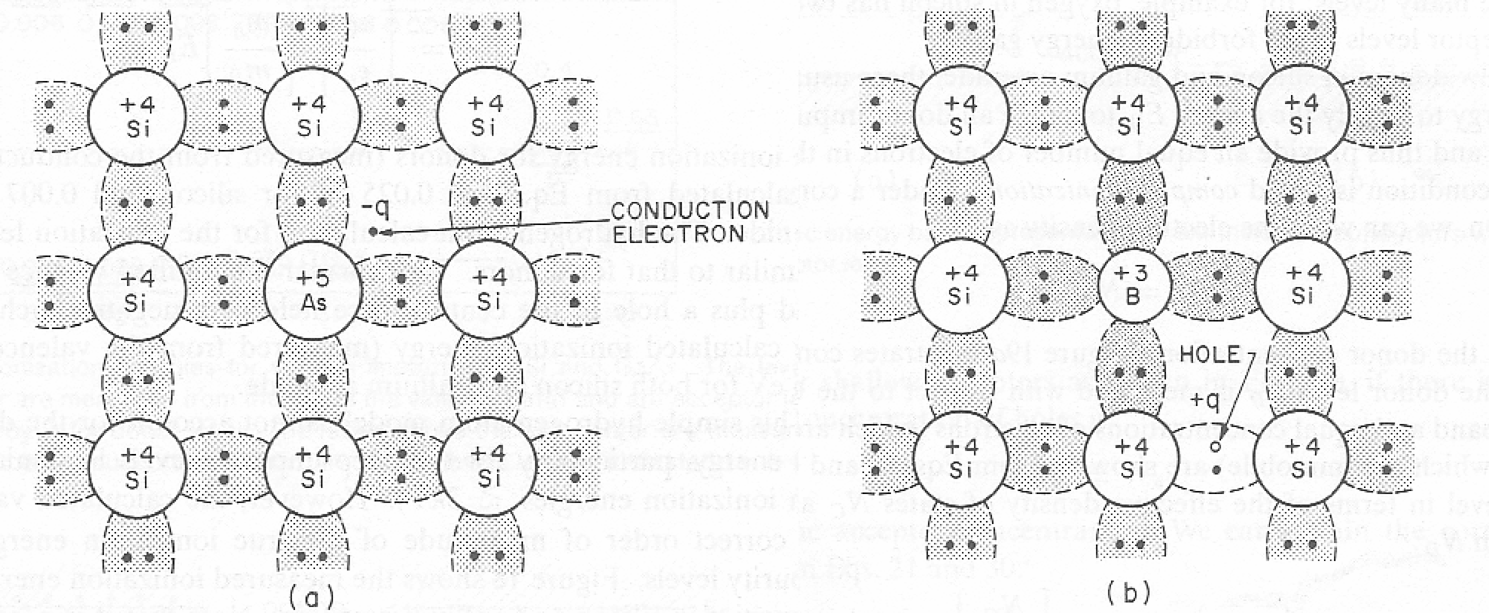


Exercise 2.2 Estimate orders of magnitude for the conductivity of Si (pure and with realistic defects)

“extrinsic” (doped) semiconductors

Donors and acceptors

- Bond model:

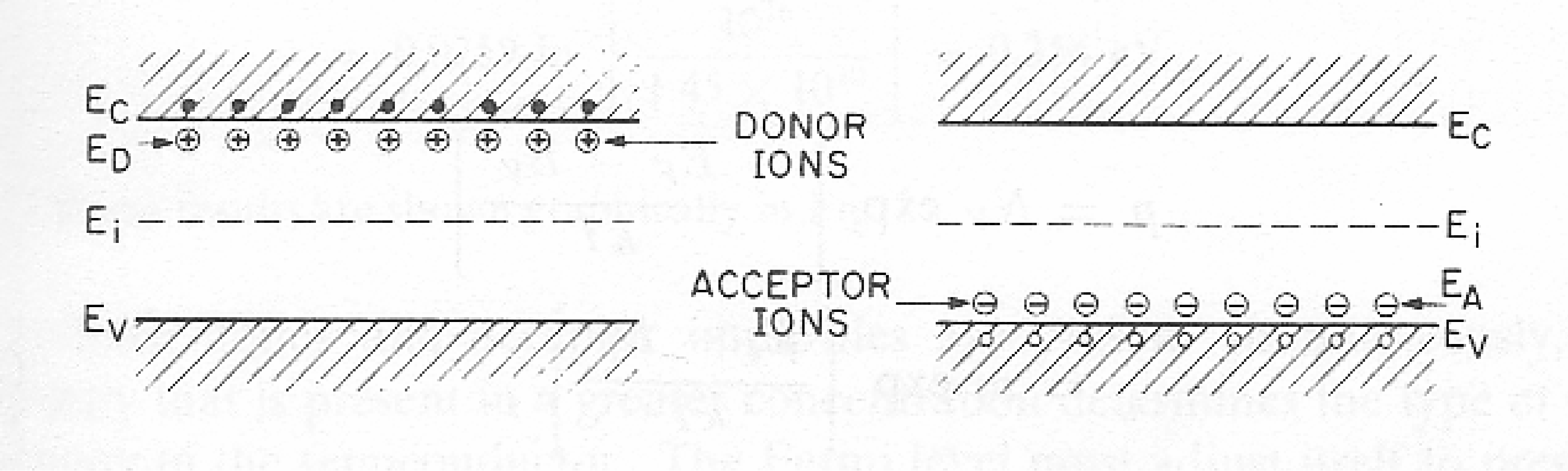


n-type Si with “*donor*” impurities
(As: 5 valence electrons)
The fifth electron is “*donated*”
to the conduction band;
the remaining positive ion is *fixed*

p-type Si with “*acceptor*” impurities
(B: 3 valence electrons)
An additional electron is “*accepted*”
from the valence band, creating a hole
The resulting negative ion is *fixed*

Donors and acceptors

- Energy band model



n-type Si with "*donor*" energy levels very close to the conduction band; ionization energy is very small, most donor atoms are ionized already at room temperature !

p-type Si with "*acceptor*" energy levels very close to the valence band; most acceptor atoms capture an electron, leaving a free hole already at room temperature !

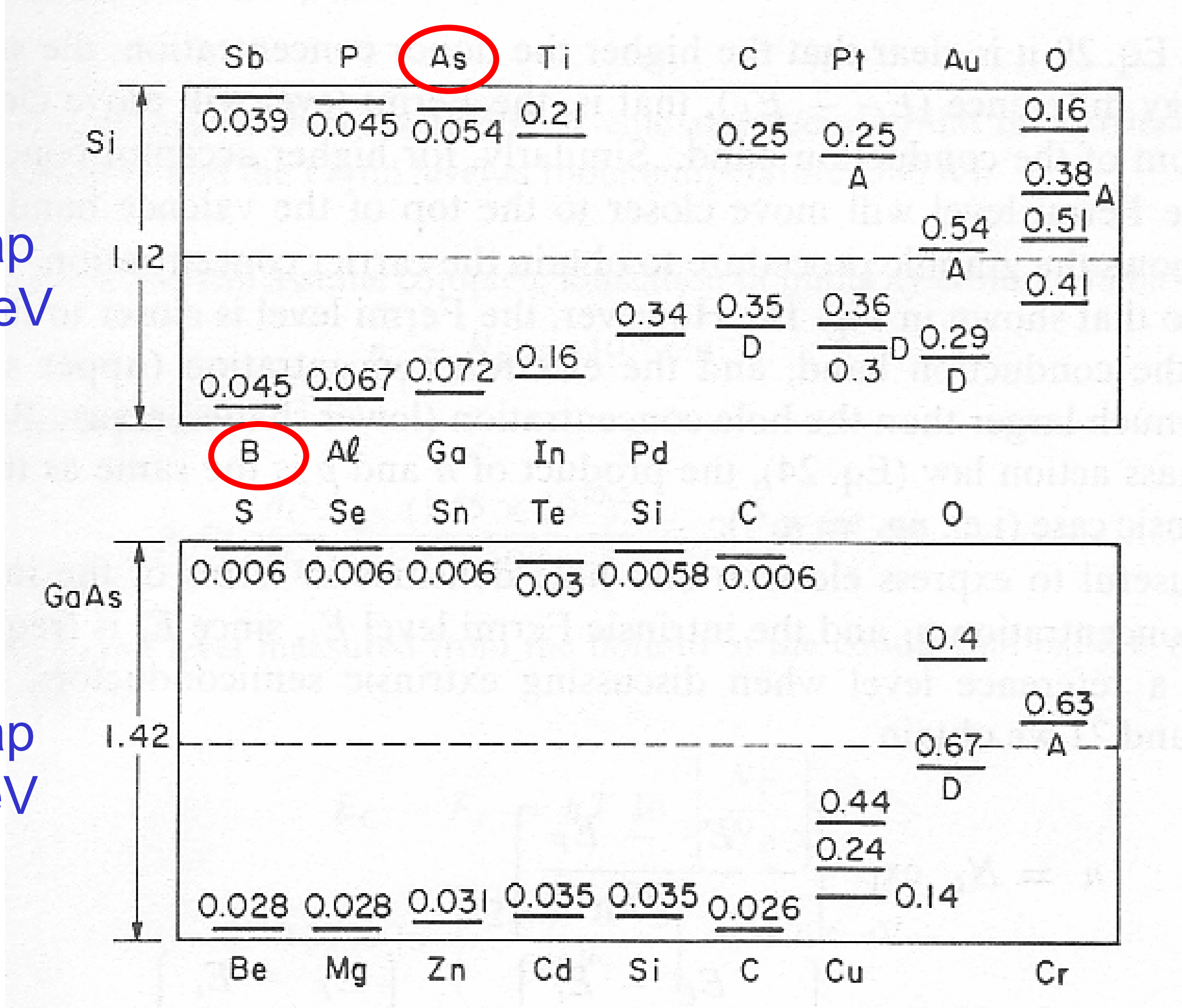
Impurities and ionization energies - 1

A = Acceptor
D = Donor

- Measured ionization energies (eV)

Si
energy gap
E_g = 1.12eV

GaAs
energy gap
E_g =1.42eV



E_C
E_C-E (eV)

E-E_V (eV)
E_V

E_C
E_C-E (eV)

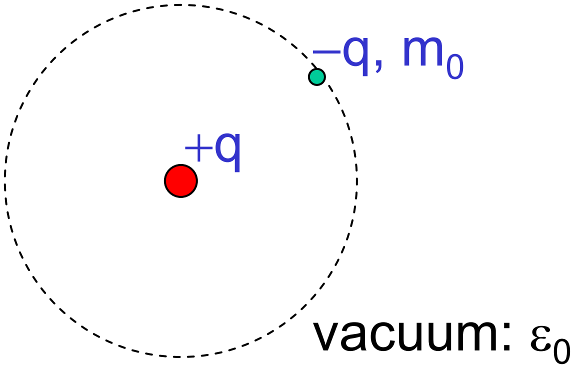
E-E_V (eV)
E_V

Impurities and ionization energies - 2

- Doping with donors (n-type)
  - For instance: P or As in Si
  - Level close to E_C
- Doping with acceptors (p-type)
  - For instance: B in Si
  - Level close to E_V
- Unwanted impurities
  - Many impurities (unavoidable, to some extent) contribute levels close to the center of the gap
  - Also these levels are important, as “traps” or “recombination-generation centers” (more on this later)

Impurities and ionization energies - 3

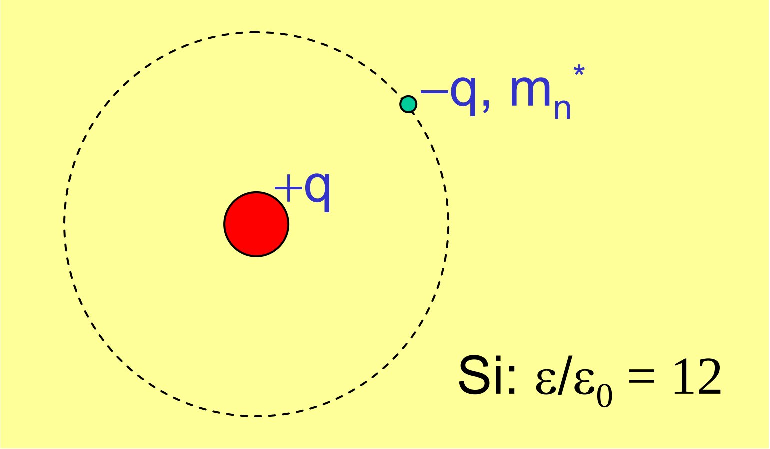
- Donor ionization energies (eV): can we understand or at least guess the order of magnitude in simple terms? Bohr model…



isolated H atom, lowest level:
Bohr model, n=1

$$E_n = -\frac{m_0 q^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} = -13.6\frac{1}{n^2}\ \text{eV}$$

$E_1 = -13.6\ \text{eV}$ ionization energy



Donor atom in Si crystal:
Lowest level for the external electron

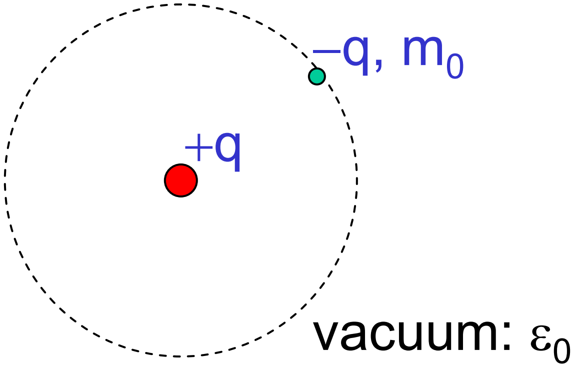
$$E_{D,n} = -\frac{m_n^* q^4}{8\varepsilon^2 h^2}\frac{1}{n^2} = \left(\frac{\varepsilon_0}{\varepsilon}\right)^2\left(\frac{m_n^*}{m_0}\right)E_{H,n}$$

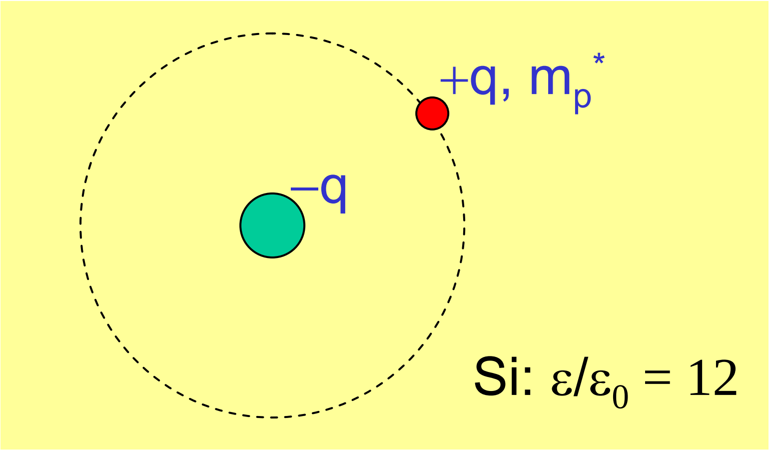
$$E_{D,1} \approx 13.6\ \text{eV}\times\frac{1}{12^2}\times 0.9 \approx 0.085\ \text{eV}$$

ionization energy

Impurities and ionization energies - 4

- Acceptor ionization energies (eV): similar reasoning





isolated H atom, lowest level:
Bohr model, n=1

$$E_n = -\frac{m_0 q^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} = -13.6\frac{1}{n^2}\ \text{eV}$$

$$E_1 = -13.6\ \text{eV}$$ ionization energy

Acceptor atom in Si crystal:
Lowest level for the hole

$$E_{D,n} = -\frac{m_p^* q^4}{8\varepsilon^2 h^2}\frac{1}{n^2} = \left(\frac{\varepsilon_0}{\varepsilon}\right)^2\left(\frac{m_p^*}{m_0}\right)E_{H,n}$$

$$E_{D,1} \approx 13.6\ \text{eV} \times \frac{1}{12^2} \times 0.19 \approx 0.018\ \text{eV}$$ ionization energy

Impurities and ionization energies - 5

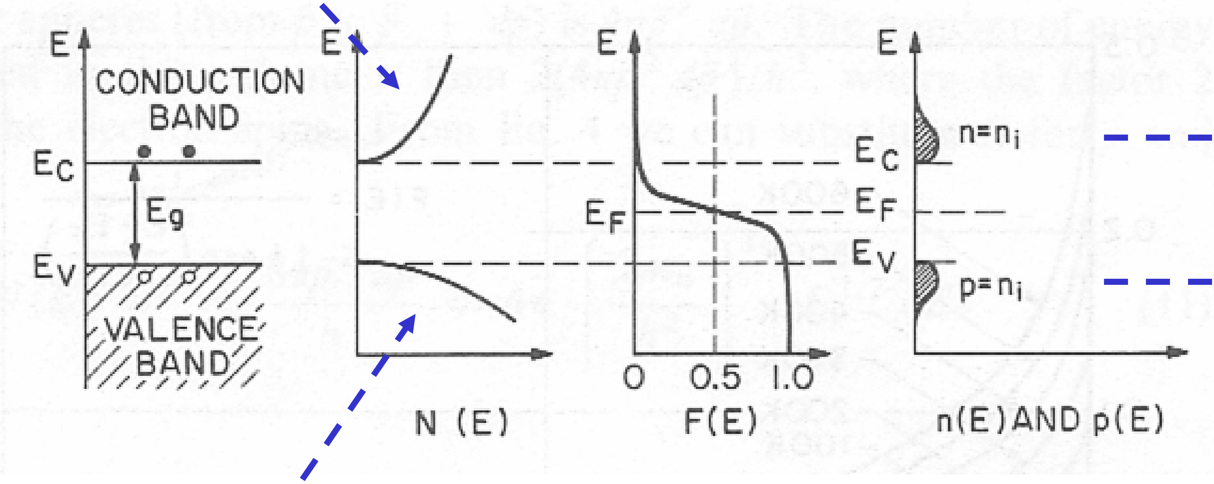
- The simple Bohr model for donor and acceptor ionization energies:
  - Describes the impurities in an oversimplified way (pseudo-hydrogen atoms with outer electron or hole orbiting through the semiconductor material):
    - Effective mass m_n^*, m_p^*
    - Dielectric constant ε
  - Gives the correct orders of magnitude for ionization energies ($E_I < 0.1$eV): OK because many semiconductor atoms are included in the Bohr orbit corresponding to the lowest level (easily checked by computing the Bohr radius)
  - Is not supposed to be able to reproduce the details !
- Small ionization energy $\Rightarrow$ most donor/acceptor atoms are ionized at room temperature

Intrinsic carrier concentration

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

$$F(E) \cong e^{-(E-E_F)/kT}$$

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



$$n \cong N_C e^{-(E_F - E_C)/kT}$$

$$p \cong N_V e^{-(E_V - E_F)/kT}$$

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

$$1 - F(E) \cong e^{-(E_F - E)/kT}$$

$$g_V(E) = \frac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3}$$

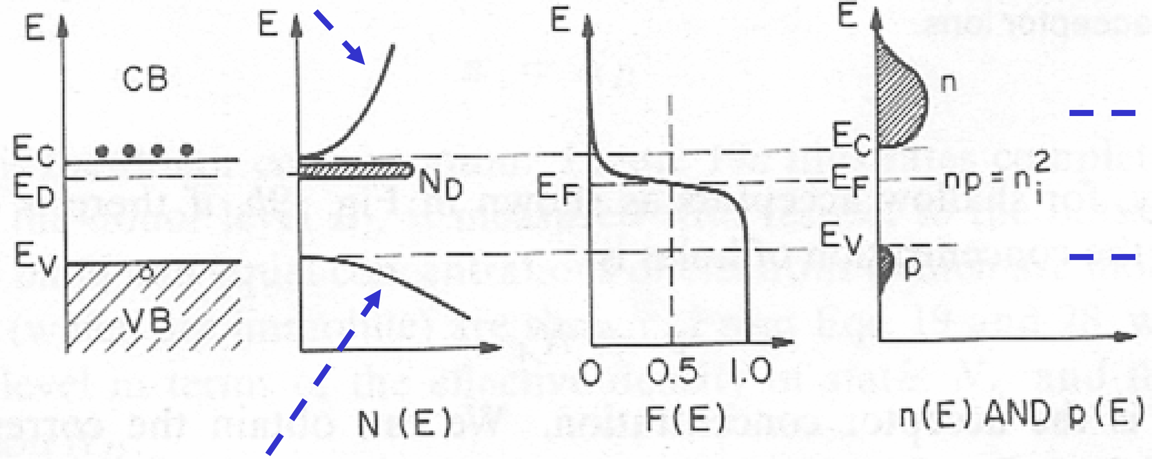
Extrinsic carrier concentration

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

The same ingredients…

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

$$F(E) \cong e^{-(E - E_F)/kT}$$



$$n \cong N_C e^{-(E_F - E_C)/kT}$$

$$p \cong N_V e^{-(E_V - E_F)/kT}$$

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

$$1 - F(E) \cong e^{-(E_F - E)/kT}$$

$$g_V(E) = \frac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3}$$

…the same (formal) results !

But now $n \neq p$: why ??

Carrier concentrations: intrinsic

- (approximate) equations valid for both intrinsic and extrinsic:

$$n \cong N_C e^{-(E_C - E_F)/kT} \qquad N_C \equiv 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$$

$$p \cong N_V e^{-(E_F - E_V)/kT} \qquad N_V \equiv 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}$$

$$\boxed{\begin{aligned} N_C &= n_i e^{(E_C - E_i)/kT} \\ N_V &= n_i e^{(E_i - E_V)/kT} \end{aligned}}$$

- Intrinsic case ($E_F = E_i$)

$$\boxed{n = p = n_i} = N_C e^{-(E_C - E_i)/kT} = N_V e^{-(E_i - E_V)/kT}$$

$$E_F = E_i = \ldots \approx \frac{E_C + E_V}{2}$$

$$\boxed{np = n_i^2} = N_C N_V e^{-(E_C - E_V)/kT} \quad \Rightarrow n_i = \sqrt{N_C N_V}\, e^{-E_g/2kT}$$

Carrier concentrations: extrinsic

- (approximate) equations valid for both intrinsic and extrinsic:

$$n \cong N_C e^{-(E_C - E_F)/kT} \qquad N_C \equiv 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2} \qquad N_C = n_i e^{(E_C - E_i)/kT}$$

$$p \cong N_V e^{-(E_F - E_V)/kT} \qquad N_V \equiv 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2} \qquad N_V = n_i e^{(E_i - E_V)/kT}$$

- Extrinsic case: $n \neq p \Leftrightarrow E_F \neq E_i$

$$n = n_i e^{(E_C - E_i)/kT} e^{-(E_C - E_F)/kT} = n_i e^{(E_F - E_i)/kT}$$

$$p = n_i e^{(E_i - E_V)/kT} e^{-(E_F - E_V)/kT} = n_i e^{(E_i - E_F)/kT}$$

E_F moves away from E_i

$$\boxed{np = n_i^2}$$

$$\boxed{\begin{array}{lll} n\text{-type}: & n \approx N_D & p \approx n_i^2 / N_D \\ p\text{-type}: & p \approx N_A & n \approx n_i^2 / N_A \end{array}}$$

approximate for complete ionization

Fermi level for complete ionization

- Complete ionization of donors:

$$n = N_C e^{-(E_C - E_F)/kT} \approx N_D \quad \Rightarrow \frac{N_C}{N_D} = e^{(E_C - E_F)/kT}$$

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

- Complete ionization of acceptors:

$$p = N_V e^{-(E_F - E_V)/kT} \approx N_A \quad \Rightarrow \frac{N_V}{N_A} = e^{(E_C - E_F)/kT}$$

$$\Rightarrow E_F - E_V = kT \ln\left(\frac{N_V}{N_A}\right)$$

Concentrations and E_F : an example

- A silicon ingot is doped with As ($N_D \approx 10^{16}$ atoms/cm^3). Find the carrier concentration and the Fermi level at room temperature (T=300K)

Assuming complete ionization of donors:

$$n \approx N_D = 10^{16}\,\mathrm{cm}^{-3}$$

$$n_i = N_C e^{-(E_C - E_i)/kT} \approx$$

$$\approx \left(2.8\times10^{19}\right)\times\left(5.2\times10^{-10}\right) \approx$$

$$\approx 1.45\times10^{10}\,\mathrm{cm}^{-3}$$

$$p \approx n_i^2 / N_D = \frac{\left(1.45\times10^{10}\right)^2}{10^{16}} =$$

$$= 2.1\times10^{4}\,\mathrm{cm}^{-3}$$

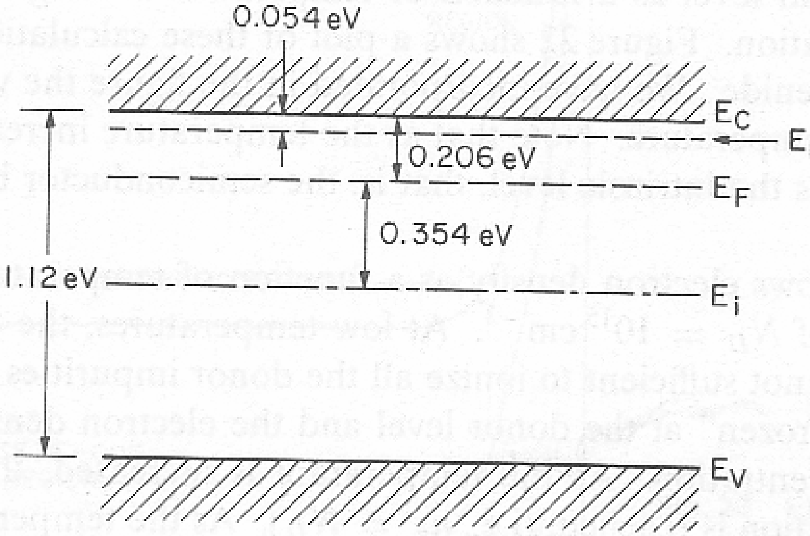


Fig. 21 Band diagram showing Fermi level E_F and intrinsic Fermi level E_i.

$$E_C - E_F = kT \ln\left(\frac{N_C}{N_D}\right) = 0.0259 \ln\left(\frac{2.8\times10^{19}}{10^{16}}\right) =$$

$$= 0.206\ \mathrm{eV}$$

$$n = n_i e^{(E_F - E_i)/kT} \Rightarrow E_F - E_i = kT \ln\left(\frac{n}{n_i}\right)$$

$$E_F - E_i = 0.0259 \ln\left(\frac{10^{16}}{1.45\times10^{10}}\right) = 0.354\ \mathrm{eV}$$

Fermi level: general case

- Both donor and acceptor impurities present simultaneously
  - Concentrations: N_D and N_A respectively
- starting point: overall *charge neutrality* and *mass action law*

$$n + N_A = p + N_D \qquad np = n_i^2$$

n-type: $N_D > N_A$

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

$$p_n = n_i^2 / n_n$$

$$\text{if} \quad |N_D - N_A| >> n_i$$

$$n_n \approx N_D - N_A$$

p-type: $N_A > N_D$

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

$$n_p = n_i^2 / p_p$$

$$\text{if} \quad |N_D - N_A| >> n_i$$

$$p_p \approx N_A - N_D$$

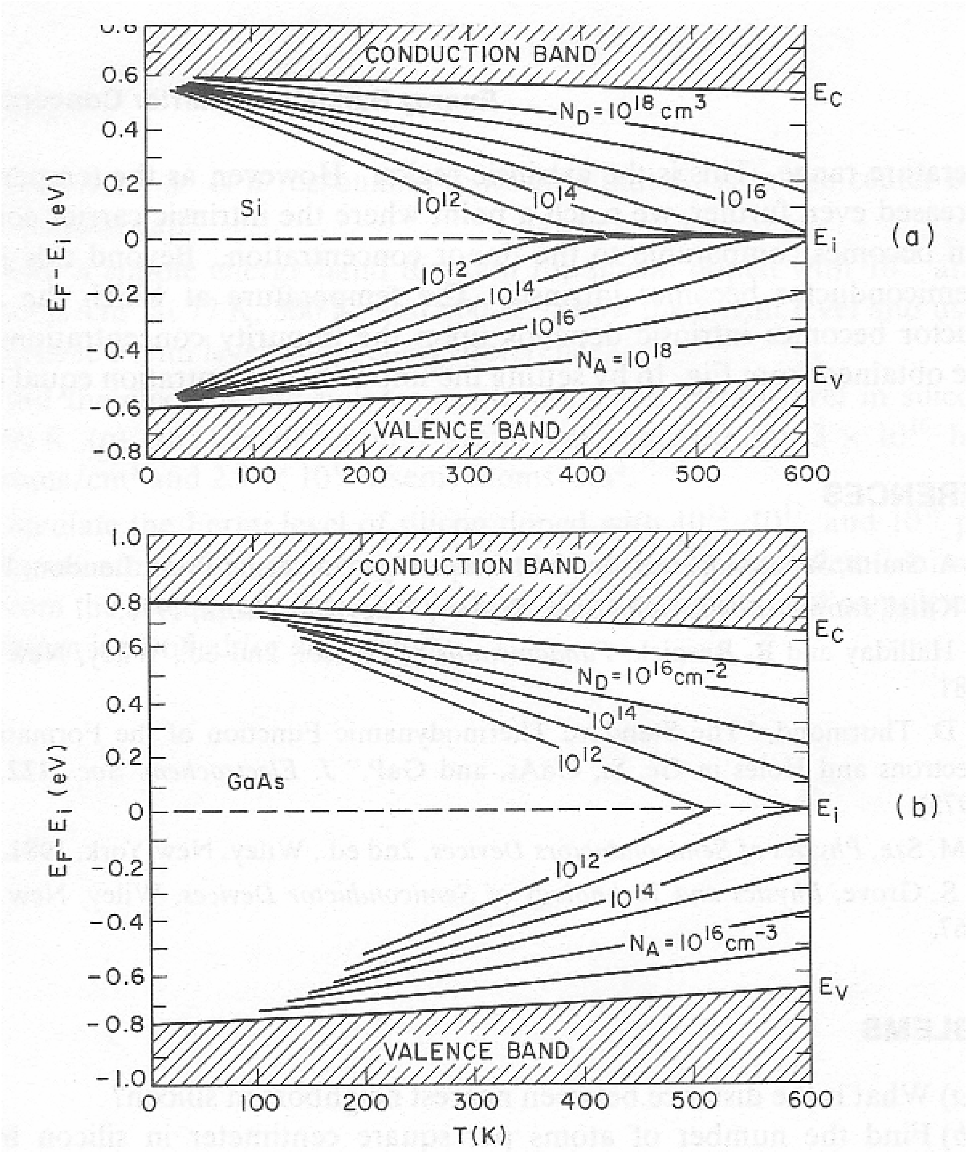
Extrinsic Fermi level vs temperature

- Fermi level computation in the general case, taking T into account:
  - from N_D and N_A compute n, p
  - from n, p extract E_F

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

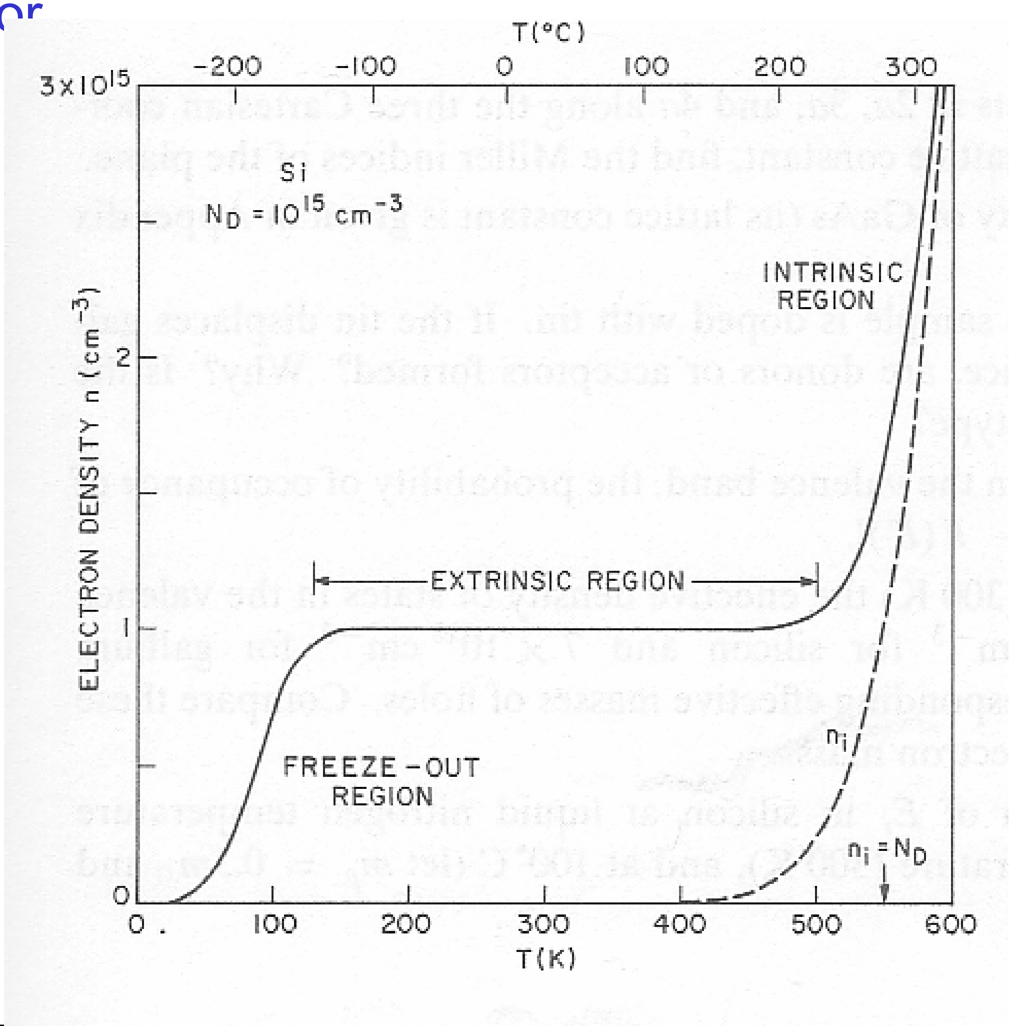
$$p = n_i e^{(E_i - E_F)/kT} \Rightarrow E_F = \dots$$

- n_i increases with T !
  - Low T: extrinsic behaviour
  - High T: intrinsic behaviour



Electron density vs temperature

- Another point of view: carrier density in n-type semiconductor
  - Very low T:
    - “freeze-out” region
    - donors not ionized
  - Medium T:
    - “extrinsic” region
    - $n \approx N_D$
  - High T:
    - “intrinsic” region
    - $n \approx n_i$



Lecture 3 - summary

- The “mass action law” ($np = n_i^2$) is always valid
- The intrinsic concentration n_i increases with T
- We found relations between n, p, n_i and E_F
- In the intrinsic case $n = p = n_i$
- We have learned how to compute n, p, and E_F in the general extrinsic case (depending on N_D, N_A)
- Intrinsic/extrinsic behaviour depends on T!

Lecture 3 – Items to be understood…

- Some items that require a deeper explanation:
  - Bohr model
  - Density of states
  - Fermi distribution function
  - Energy band model
  - Donors and acceptor energy levels

Lecture 3 - Glossary

Fermi probability density function		
Fermi level		
intrinsic semiconductor		
exstrinsic semiconductors		
donor		
acceptor		
energy band model		
bond model		
electrons		
holes		
carriers		
intrinsic carrier concentrations		
extrinsic carrier concentrations		
charge neutrality		
mass action law		

Lecture 3 - exercises

- **Exercise 3.1:** A silicon sample at T=300K contains an acceptor impurity concentration of $N_A=10^{16}$ cm^{-3}. Determine the concentration of donor impurity atoms that must be added so that the silicon is n-type and the Fermi energy is 0.20 eV below the conduction band edge.
- **Exercise 3.2:** Find the electron and hole concentrations and Fermi level in silicon at 300K (a) for $1\text{x}10^{15}$ boron atoms/cm^3 and (b) for $3\text{x}10^{16}$ boron atoms /cm^3 together with $2.9\text{x}10^{16}$ arsenic atoms/cm^3.
- **Exercise 3.3:** Calculate the Fermi level of silicon doped with 10^{15}, 10^{17} and 10^{19} phosphorus atoms/cm^3, assuming complete ionization. From the calculated Fermi level, check if the assumption of complete ionization is justified for each doping. Assume that the ionized donors density is given by $N_D^+ = N_D(1-F(E_D))$.

Backup slides