Chapter 2

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Bonding forces

- Ionic (example: NaCl)
  - Sodium gives an electron to chlorine, this leads to Na^+
  - Chlorine accepts an electron from sodium, this leads to Cl^-
  - Electro static charge pulls the atoms together until balanced by repulsive charges
  - Outer orbits are all filled, thus atoms are tightly bound, thus NaCl is a good insulator

Bonding forces

- Metallic
  - The ions are embedded in a sea of free electrons (there are more electrons than places to put electrons-states).
  - The bonding is between the positive ions cores and the surrounding free electrons.
  - This is a complex relationship as can be seen from the widely varying melting points of various metals.

Bonding forces

- Pauli exclusion principle: **No two electrons in an interacting system can have the same quantum numbers.**
  - An **interacting system** is one in which electron wave functions overlap.
  - An electron's **quantum number** describes which **state** it is in.
    - A **state** is a valid place for an electron to occupy.
- We need the Pauli exclusion principle to understand covalent bonding.

Bonding forces

- Covalent
  - Diamond lattice structure (Ge, Si, C)
  - Each atom has 4 neighbors.
  - Each atom shares its electrons with its neighbors.
  - Each bond is composed of two electrons with different spins.
  - Therefor there are no free electrons, thus Si and Ge are insulators at 0K. (What about at higher temperatures?)

Bonding forces

- Covalent/Ionic
  - Zincblende lattice structure (GaAs, InP, ZnSe)
  - Each atom has 4 neighbors that are not of the same type, thus there is ionic bonding
  - Each atom shares some of its electrons with its neighbors, thus there is covalent bonding.
  - The bonding is mixed between ionic and covalent and in general becomes more ionic as you separate across the periodic table(III-V to II-VI).

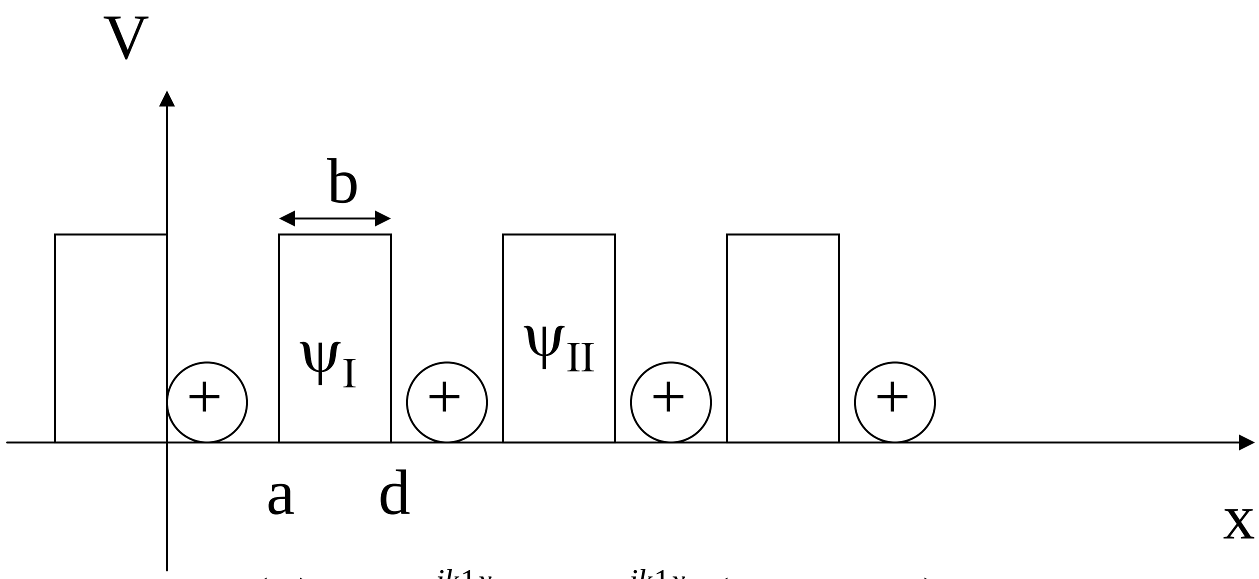
Energy bands

- As atoms are brought closer together their electron wave functions start to interact.
- Two atoms brought close together will see each energy level split into two, three atoms will see a split of three and so on
- A very large amount of atoms will see these discrete levels smear into a band of energy levels.

Energy bands

- These bands of states are separated by forbidden regions.
- The lowest unfilled band is the conduction band (at 0K in semiconductors).
- The highest filled band is the valence band (at 0K in semiconductors).

Energy bands



$$\psi_I(x) = Ae^{ik1x} + Be^{-ik1x}, (0 \le x \le a)$$

$$\frac{\hbar^2 k_1^{\,2}}{2m} = E$$

$$\psi II(x) = Ce^{ik2x} + De^{-ik2x}, (a \le x \le a + b = d)$$

$$\frac{\hbar^2 k_2^{\,2}}{2m} = E - V$$

Energy bands

- The function must repeat itself
- The wavefunctions at the boundaries must be equal to each other.
- The derivatives of the wavefunctions at the boundaries must be equal to each other.

Energy bands

- This leads to a system of four equations and four unknowns. If the determinant of this system equals zero then there is a non-trivial solution. After a bit of algebra this leads to the dispersion relation.

Energy bands (Dispersion relation)

$$(E > V)$$

$$\cos k_1 a \cos k_2 b - \frac{{k_1}^2 + {k_2}^2}{2k_1 k_2} \sin k_1 a \sin k_2 b = \cos kd$$

$$\frac{\hbar^2 {k_1}^2}{2m} = E, \frac{\hbar^2 {k_2}^2}{2m} = E - V$$

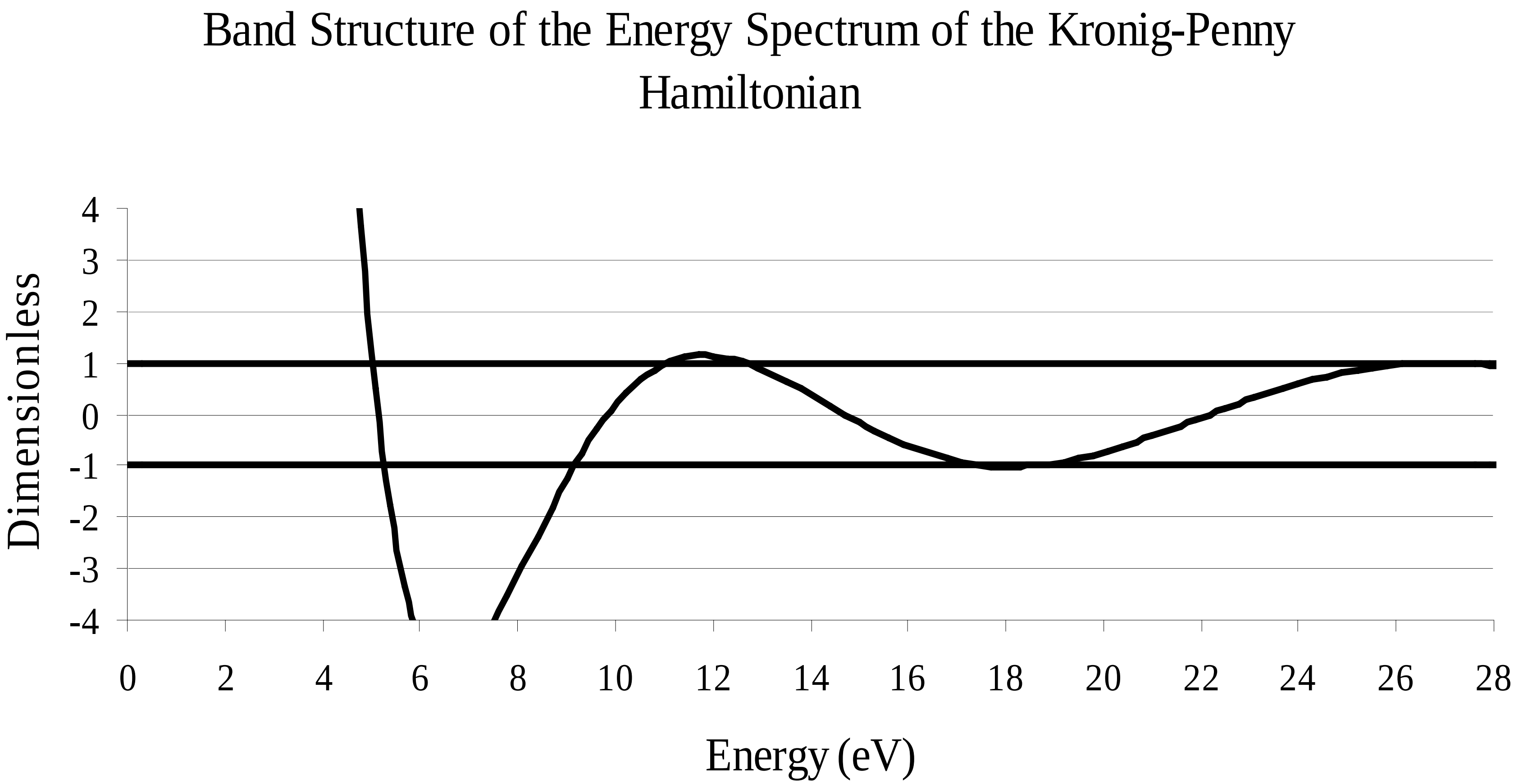
$$(E < V)$$

$$\cos k_1 a \cosh \kappa b - \frac{{k_1}^2 - \kappa^2}{2k_1 \kappa} \sin k_1 a \sinh \kappa b = \cos kd$$

$$\frac{\hbar^2 {k_1}^2}{2m} = E, \frac{\hbar^2 \kappa^2}{2m} = V - E$$

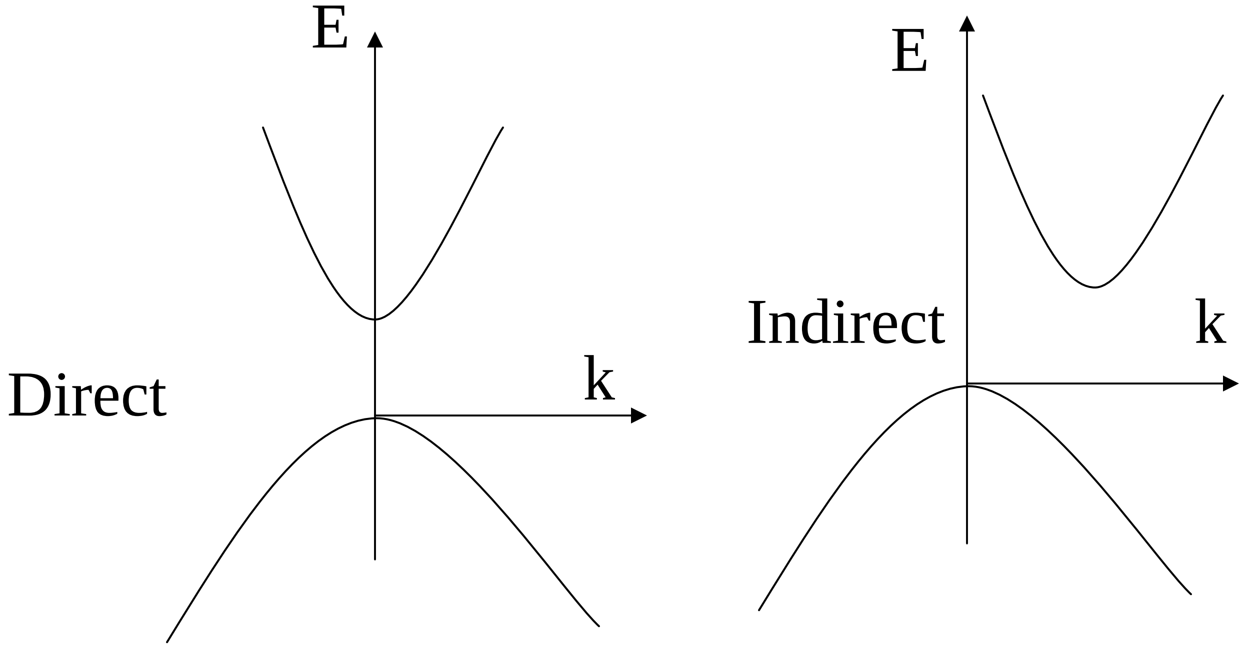
Energy bands

d=5.45Å
a=1.1Å
V=8eV



Energy Bands

- If you plot the allowed values of energy vs. the propagation constant you get the band structure shown:



Energy Bands

- Insulator (large band gap) hard to move an electron from the valence to the conduction band at any temperature.
- Semiconductor (small band gap optical photons and heat (lattice vibrations) can easily give the required energy to move to the conduction band
- Metals (band gaps overlap), partially filled, easy for current to flow

Energy bands

- The inter-atomic spacing varies with the direction you are moving in the crystal {111}planes would have a smaller d than {100} planes, thus the energy gaps are different in each direction.
- This gives rise to different bands, but usually effect due to this can be averaged.

Charge carriers in semiconductors

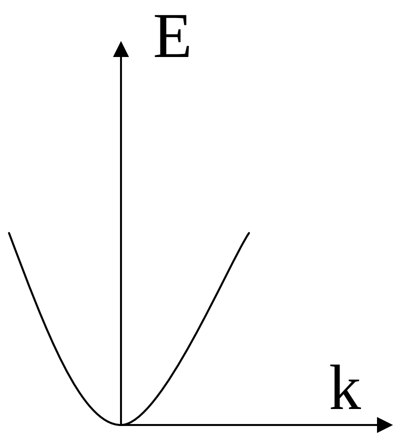
- Electrons and holes
  - Electrons (e) we know about, but what is a hole (h)?
    - When an electron receives enough energy to jump from the valence band to the conduction band it leaves behind an empty state. This creates an electron-hole pair (EHP)
    - Hole current is really due to an electron moving in the opposite direction in the valence band.
    - Electron current is an electron moving from state to state in the conduction band.

Charge carriers in semiconductors

- Effective mass
  - Electrons in a crystal are not totally free.
  - The periodic crystal affects how electrons move through the lattice.
  - We use and effective mass to modify the mass of an electron in the crystal and then use the E+M equations that describe free electrons.

Charge carriers in semiconductors

- Effective mass



$$p = mv = \hbar k$$

$$E = \frac{1}{2}mv^2 = \frac{\hbar^2}{2m}k^2$$

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m}$$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

Charge carriers in semiconductors

- Effective mass
  - The double derivative of E is a constant
  - Not all semiconductors have a perfectly parabolic band structure
    - This gives rise to different effective masses in different crystal directions. This can be compensated by using an average value of effective mass.

Charge carriers in semiconductors

- Effective mass (for density of states calculation)

	Ge	Si	GaAs
m_n^*	$0.55\ m_0$	$1.1\ m_0$	$0.067\ m_0$
m_p^*	$0.37\ m_0$	$.56\ m_0$	$0.48\ m_0$

Charge carriers in semiconductors

- Intrinsic material
  - A perfect semiconductor crystal
    - no impurities or defects
  - No charge carriers at 0K
    - valence band is filled, conduction band empty
  - Heat (lattice vibrations can break a covalent bond and push an electron into the conduction band (EHP)
  - This electron is moving several lattice constants away in a QM probability distribution.

Charge carriers in semiconductors

- Intrinsic material
  - Each electron pumped up to the valence band leaves an empty state behind, thus for intrinsic material the electron concentration in the conduction band (n e/cm^3)=the hole concentration in the valence band (p h/cm^3)

$$n = p = n_i$$

Charge carriers in semiconductors

- Intrinsic material
  - If this relation is to hold then the generation rate of EHP's must equal the recombination rate of EHP's

$$n = p = n_i$$

$$r_i = g_i$$

$$r_i = \alpha_r n_0 p_0 = \alpha_r n_i^{2} = g_i$$

Charge carriers in semiconductors

- Extrinsic material
  - Intrinsic material is not very useful except for devices which change their conductivity based on optical or thermal excitation. There is no gain mechanism involved and thus large areas are needed to detect the effect, thus are slow.
  - One can create extrinsic material by replacing semiconductor atoms in the lattice with atoms from different groups in the periodic table.

Charge carriers in semiconductors

- Extrinsic material.

II	III	IV	V	VI
	B	C		
	Al	Si	P	S
Zn	Ga	Ge	As	Se
Cd	In		Sb	Te

Charge carriers in semiconductors

- Extrinsic material.
  - Elements from group V give rise to energy levels close the the conduction band in Si and Ge and is completely filled at 0K. It only takes a little energy to make an electron jump from this level to the conduction band. This new energy level donates an electron and so group V elements are know as donors (with respect to Si and Ge)

Charge carriers in semiconductors

- Extrinsic material.
  - Elements from group III give rise to energy levels close the the valence band in Si and Ge and is completely empty at 0K. It only takes a little energy to make an electron jump from the valence band to this new level. This new energy level accepts an electron and so group III elements are knows as acceptors (with respect to Si and Ge)

Charge carriers in semiconductors

- Extrinsic material.
  - Not all group III and V elements make good dopant sources, if the new energy level is near the middle of the band gap then it takes more energy to accept or donate an electron.
  - In III-VI semiconductors it is more complex
    - group VII elements on a VI site will donate an electron
    - group II elements on a III site will accept an electron
    - group IV elements can go on either a III or VI and thus are amphoteric

Charge carriers in semiconductors

- Electrons and holes in a quantum well
  - A quantum well consists of a thin (~100Å) semiconductor layer sandwiched between two semiconductor layers with larger band gaps.
  - In the one dimensional case this gives rise to discrete energy levels above the conduction band and below the valence band.
  - This well serves as a trap for EHP's and when an EHP recombines in a direct band semiconductor, a photon is emitted.

Charge carriers in semiconductors

- Electrons and holes in a quantum well
  - This trapping effect increases the probability of an electron hole pair recombining between these new energy levels compared to the bulk semiconductor. This leads to more efficient lasers due to the fact that the energy spread of the photons generated is tighter than compared to bulk material.

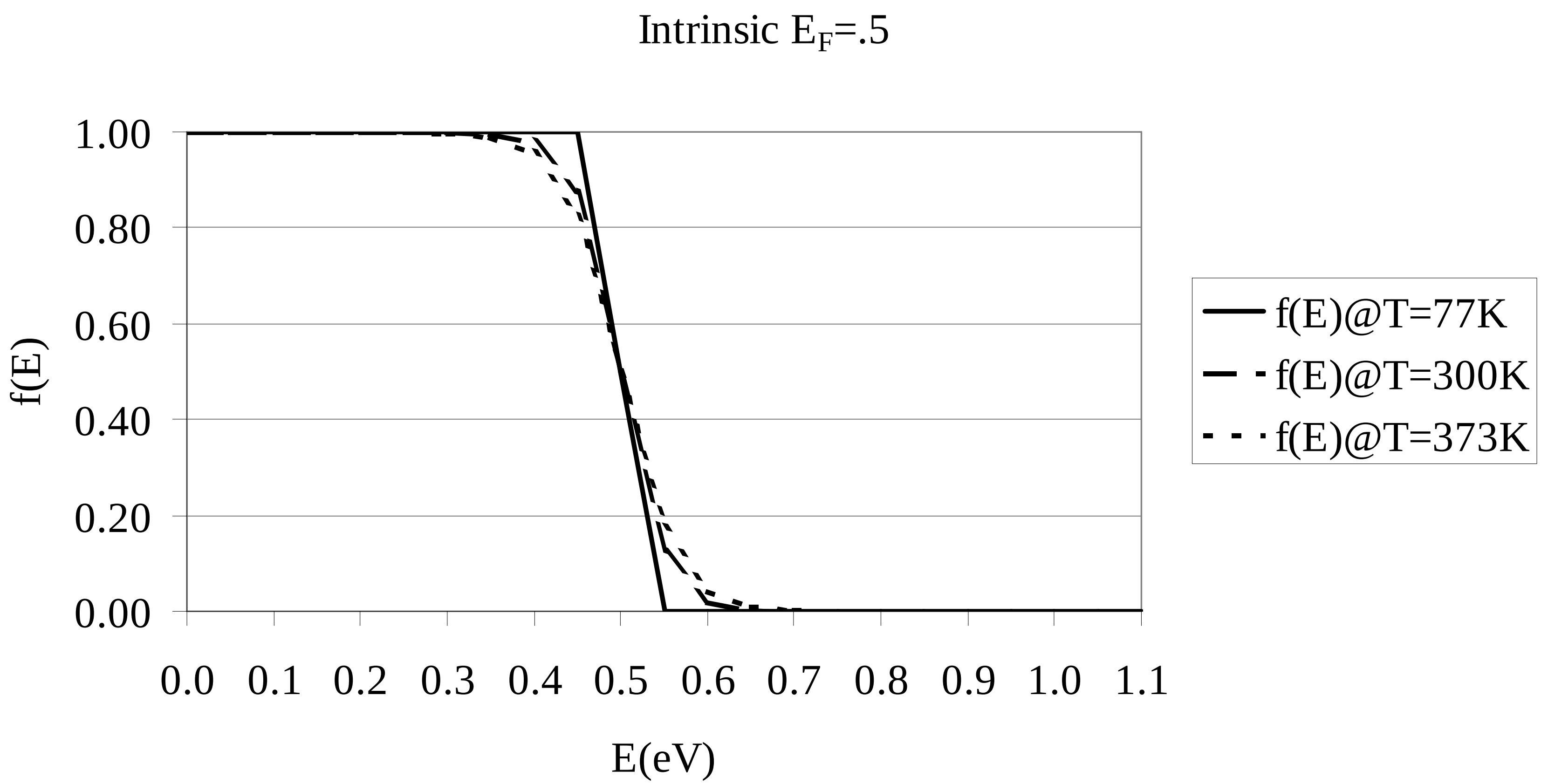
Carrier concentrations

- The Fermi level
  - Indistinguishability of electrons
  - Wave nature of electrons
  - Pauli exclusion principle

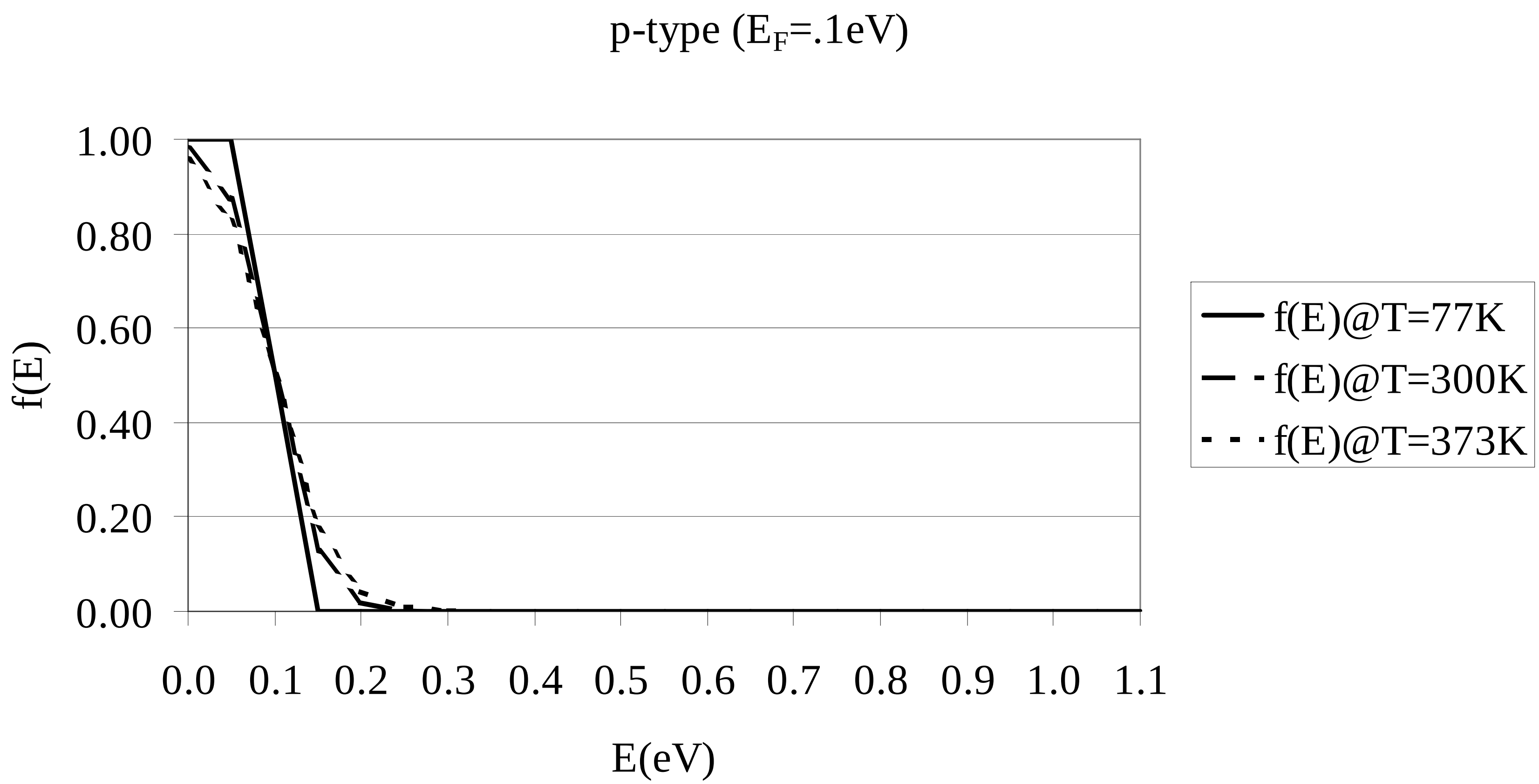
$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

$$f(E_F) = \frac{1}{1+1} = \frac{1}{2}$$

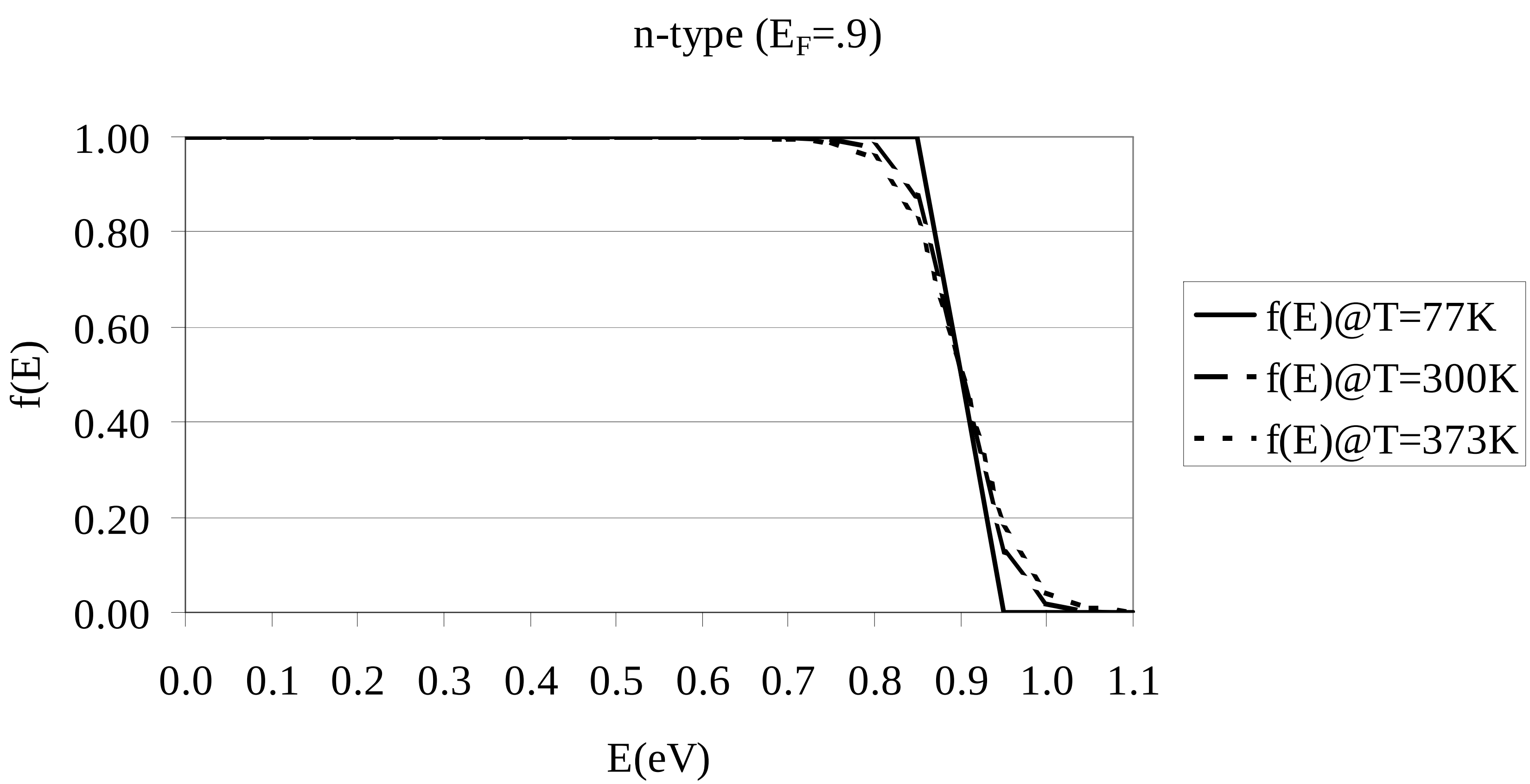
Carrier concentrations



Carrier concentrations



Carrier concentrations



Carrier concentrations

- The Fermi distribution only shows the probability of an available state being filled it does not allow states to form.
- The probability of a state being filled with an electron is f(E).
- The probability of a state being empty
  1- f(E) (probability of finding a hole).

Carrier concentrations

$$n_o = N_C f(E_c)$$

$$f(E_c) = \frac{1}{1 + e^{(E_c - E_F)/kT}} \approx e^{-(E_c - E_F)/kT}, E_F < E_C - 2kT$$

$$n_o = N_C e^{-(E_c - E_F)/kT}$$

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

Carrier concentrations

$$p_o = N_V(1 - f(E_c))$$

$$1 - f(E_v) = 1 - \frac{1}{1 + e^{(E_V - E_F)/kT}} \approx e^{-(E_F - E_V)/kT}, E_F > E_V + 2kT$$

$$p_o = N_V e^{(-E_F - E_v)/kT}$$

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

Carrier concentrations

$$n_o p_o = n_i^{\;2}$$

$$n_i = \sqrt{N_C N_V}\, e^{-Eg/2kT}$$

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

Carrier concentrations PE:

Calculate ni for Si at 300K

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

Carrier concentrations PE:

$$n = 2\left(\frac{2\pi * 1.38E^{-23} J/K * 300K}{(6.63E^{-34} J - s)^2}\right)^{\frac{3}{2}}$$

$$(1.1 * .56 * 9.11E^{-31} kg^2)^{\frac{3}{4}} e^{-1.11/2/.0259}$$

$$n_i = 2(5.91771E^{46} / J - s^2)^{\frac{3}{2}} (5.112E^{-61} kg^2)^{\frac{3}{4}} e^{-21.236}$$

$$n_i = 2 * 1.4396E^{70} \frac{1}{kg^{3/2} m^3} * 6.04593E^{-46} kg^{3/2} * 5.99143E^{-10}$$

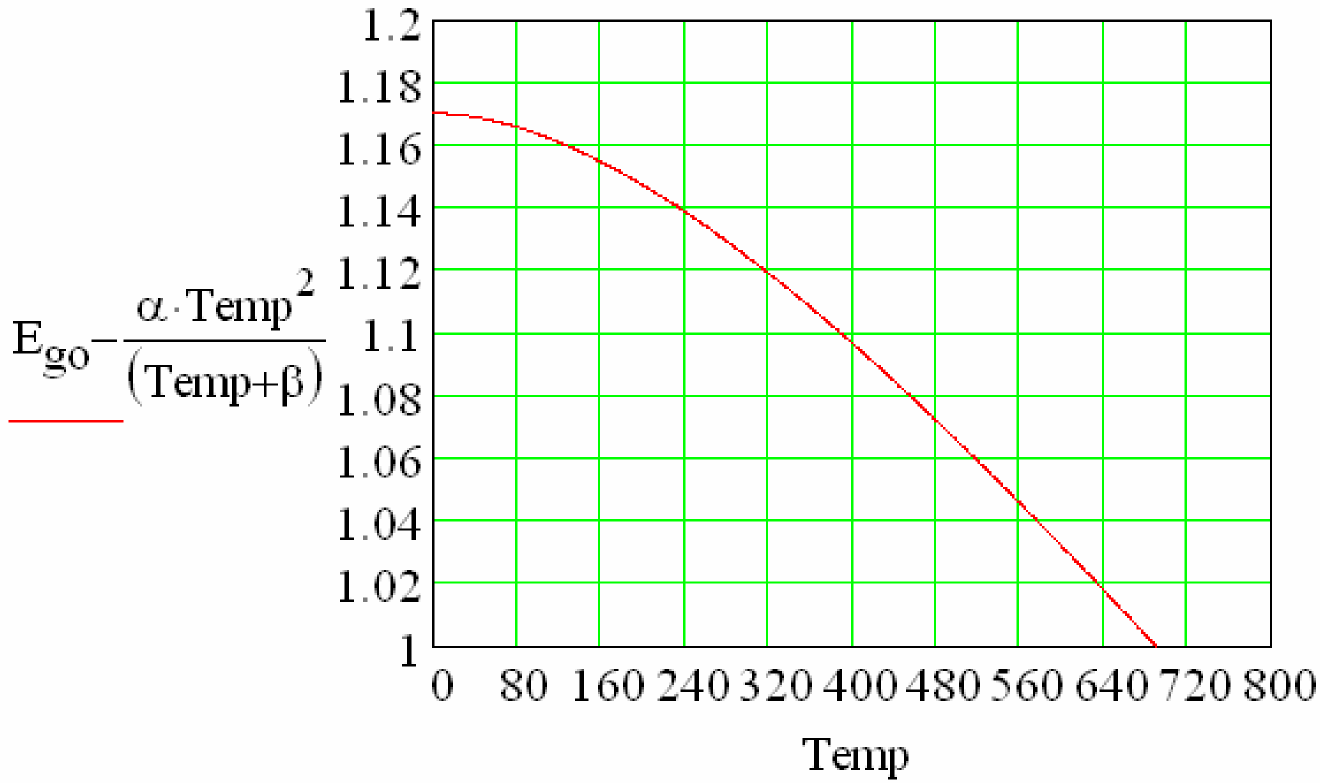
$$n_i = 1.043E^{16} m^{-3} = 1.043E^{10} cm^{-3}$$

Carrier concentrations

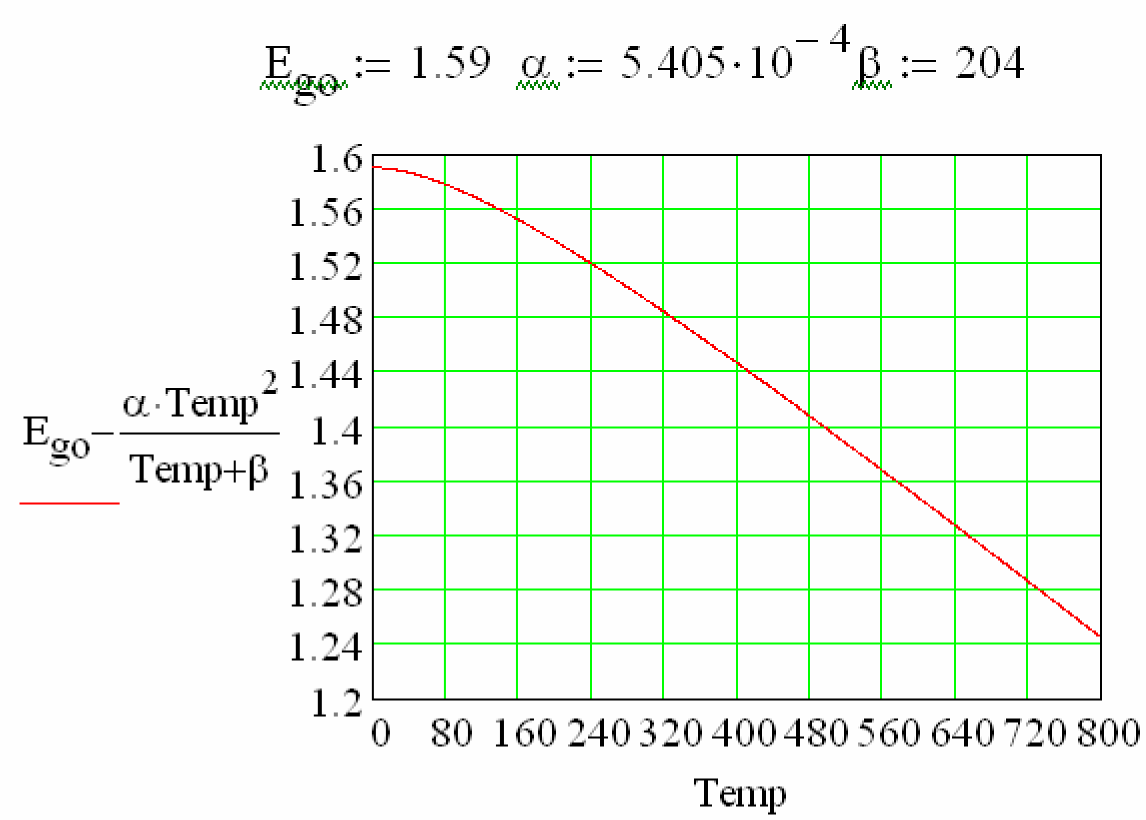
- Space charge neutrality
  - $p_o + N_d^+ = n_o + N_a^-$
  - no = $N_d^+ - N_a^-$, for strongly n-type
  - po = $N_a^- - N_d^+$, for strongly p-type

The Band Gap varies with Temperature (Si)

$$E_{go} := 1.17 \quad \alpha := 4.73\cdot 10^{-4} \quad \beta := 636$$



The Band Gap varies with Temperature (GaAs)



What is Ei for Si for 300K?

$$Temp := 300$$

$$E_{go} := 1.17 \qquad \alpha := 4.73\cdot 10^{-4} \qquad \beta := 636$$

$$E_g := E_{go} - \frac{\alpha\cdot Temp^2}{Temp + \beta} \qquad E_g = 1.125$$

$$N_C := 2.86\cdot 10^{19} \qquad N_V := 2.66\cdot 10^{19}$$

$$N_{CTemp} := \frac{N_C}{300^{\frac{3}{2}}}\cdot Temp^{\frac{3}{2}}$$

$$N_{VTemp} := \frac{N_V}{300^{\frac{3}{2}}}\cdot Temp^{\frac{3}{2}}$$

$$E_C := E_g$$

$$E_i := \frac{(E_C + E_V)}{2} + \frac{k\cdot Temp}{q}\cdot \ln\left(\frac{N_{VTemp}}{N_{CTemp}}\right)$$

$$E_i = 0.56$$

What is Ei for Si for 77K?

$$Temp := 77$$

$$E_{go} := 1.17 \qquad \alpha := 4.73 \cdot 10^{-4} \qquad \beta := 636$$

$$E_g := E_{go} - \frac{\alpha \cdot Temp^2}{Temp + \beta} \qquad E_g = 1.166$$

$$N_C := 2.86 \cdot 10^{19} \qquad N_V := 2.66 \cdot 10^{19}$$

$$N_{CTemp} := \frac{N_C}{300^{\frac{3}{2}}} \cdot Temp^{\frac{3}{2}}$$

$$N_{VTemp} := \frac{N_V}{300^{\frac{3}{2}}} \cdot Temp^{\frac{3}{2}}$$

$$E_C := E_g$$

$$E_i := \frac{(E_C + E_V)}{2} + \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_{CTemp}}\right)$$

$$E_i = 0.583$$

What is Ei for Si for 400K?

$\text{Temp} := 400$

$E_{go} := 1.17 \qquad \alpha := 4.73 \cdot 10^{-4} \qquad \beta := 636$

$$E_g := E_{go} - \frac{\alpha \cdot \text{Temp}^2}{\text{Temp} + \beta} \qquad E_g = 1.097$$

$N_C := 2.86 \cdot 10^{19} \qquad N_V := 2.66 \cdot 10^{19}$

$$N_{CTemp} := \frac{N_C}{300^{\frac{3}{2}}} \cdot \text{Temp}^{\frac{3}{2}} \qquad N_{CTemp} = 4.403 \times 10^{19}$$

$$N_{VTemp} := \frac{N_V}{300^{\frac{3}{2}}} \cdot \text{Temp}^{\frac{3}{2}} \qquad N_{VTemp} = 4.095 \times 10^{19}$$

$E_C := E_g$

$$E_i := \frac{(E_C + E_V)}{2} + \frac{k \cdot \text{Temp}}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_{CTemp}}\right)$$

$E_i = 0.546$

Draw an EGB for Si ND=10^{16}, for 77K

$$Temp := 77$$

$$E_{go} := 1.17 \qquad \alpha := 4.73 \cdot 10^{-4} \qquad \beta := 636 \qquad E_i := \frac{(E_C + E_V)}{2} + \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_{CTemp}}\right)$$

$$E_g := E_{go} - \frac{\alpha \cdot Temp^2}{Temp + \beta} \qquad E_g = 1.166 \qquad E_i = 0.583$$

$$N_C := 2.86 \cdot 10^{19} \qquad N_V := 2.66 \cdot 10^{19}$$

$$N_D := 10^{16}$$

$$N_{CTemp} := \frac{N_C}{300^{\frac{3}{2}}} \cdot Temp^{\frac{3}{2}} \qquad N_{CTemp} = 3.719 \times 10^{18}$$

$$E_F := E_C - \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{CTemp}}{N_D}\right)$$

$$E_F = 1.127$$

$$N_{VTemp} := \frac{N_V}{300^{\frac{3}{2}}} \cdot Temp^{\frac{3}{2}} \qquad N_{VTemp} = 3.459 \times 10^{18}$$

$$E_C := E_g$$

Draw an EGB for Si ND=10^{16}, for 600K

$$Temp := 600$$

$$E_{go} := 1.17 \qquad \alpha := 4.73\cdot 10^{-4} \qquad \beta := 636$$

$$E_i := \frac{(E_C + E_V)}{2} + \frac{k\cdot Temp}{q}\cdot \ln\left(\frac{N_{VTemp}}{N_{CTemp}}\right)$$

$$E_g := E_{go} - \frac{\alpha\cdot Temp^2}{Temp + \beta} \qquad E_g = 1.032$$

$$E_i = 0.512$$

$$N_C := 2.86\cdot 10^{19} \qquad N_V := 2.66\cdot 10^{19}$$

$$N_D := 10^{16}$$

$$N_{CTemp} := \frac{N_C}{300^{\frac{3}{2}}}\cdot Temp^{\frac{3}{2}} \qquad N_{CTemp} = 8.089\times 10^{19}$$

$$E_F := E_C - \frac{k\cdot Temp}{q}\cdot \ln\left(\frac{N_{CTemp}}{N_D}\right)$$

$$E_F = 0.567$$

$$N_{VTemp} := \frac{N_V}{300^{\frac{3}{2}}}\cdot Temp^{\frac{3}{2}} \qquad N_{VTemp} = 7.524\times 10^{19}$$

$$E_C := E_g$$

Find the electron and hole concentrations and fermi level in Si at 300K

- Bn 10^{15}cm^{-3}
- Bn 10^{16}cm^{-3}
- As 10^{16}cm^{-3}

$$N_D := 10^{16}$$

$$E_F := E_C - \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{CTemp}}{N_D}\right)$$

$$E_F = 0.919$$

$$N_{CTemp} \cdot e^{-(E_C - E_F) \cdot \frac{q}{k \cdot Temp}} \quad n = 1 \times 10^{16}$$

$$N_A := 10^{16} \qquad E_V := 0$$

$$E_F := -E_V + \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_A}\right)$$

$$E_F = 0.204$$

$$p := N_{CTemp} \cdot e^{-(E_F - E_V) \cdot \frac{q}{k \cdot Temp}} \quad p = 1.07 \times 10$$

$$N_A := 10^{15} \qquad E_V := 0$$

$$E_F := -E_V + \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_A}\right)$$

$$E_F = 0.264$$

$$p := N_{CTemp} \cdot e^{-(E_F - E_V) \cdot \frac{q}{k \cdot Temp}} \quad p = 1.075 \times 10^{15}$$

Find the electron and hole concentrations and fermi level in Si at 300K

- Bn $10^{15}cm^{-3}$
- Bn $10^{16}cm^{-3}$
- As $10^{16}cm^{-3}$

$$N_D := 10^{16}$$

$$E_F := E_C - \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{CTemp}}{N_D}\right)$$

$$E_F = 0.919$$

$$N_{CTemp} \cdot e^{-(E_C - E_F)\cdot\frac{q}{k \cdot Temp}} \quad n = 1 \times 10^{16}$$

$$N_A := 10^{16} \qquad E_V := 0$$

$$E_F := -E_V + \frac{k \cdot Temp}{q} \cdot \ln\left(\frac{N_{VTemp}}{N_A}\right)$$

$$E_F = 0.204$$

$$p := N_{CTemp} \cdot e^{-(E_F - E_V)\cdot\frac{q}{k \cdot Temp}} \quad p = 1.075 \times 10^{16}$$

$$n \cdot p := n_i^2$$