VE320 Intro to Semiconductor Devices

Mid1 Recitation Class

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Contents

Lattice Types

- Simple cubic: #atom $= \frac{1}{8} \times 8 = 1$, $r(\text{atom}) = \frac{a}{2}$
- Body-centered cubic: #atom $= \frac{1}{8} \times 8 + 1 = 2$, $r(\text{atom}) = \frac{\sqrt{3}a}{4}$
- Face-centered cubic: #atom $= \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$, $r(\text{atom}) = \frac{\sqrt{2}a}{4}$
- Volume Density $= \frac{\#\text{atoms per unit cell}}{\text{volume of unit cell}}$
- Surface Density $= \frac{\#\text{atoms per lattice plane}}{\text{area of lattice plane}}$
- A corner atom is shared by eight unit cells so that each corner atom contributes $\frac{1}{8}$ of its volume to each unit cell.
- A surface atom is shared by two unit cells so that each surface atom contributes $\frac{1}{2}$ of its volume to each unit cell.

Miller Index
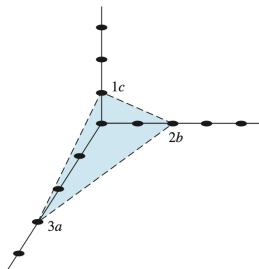
- Steps:
    - a. Find the intersection (∞ if parallel to the axis)
    - b. Write the reciprocal
    - c. Times the lowest common denominator
- All parallel planes are equivalent.
- $[hkl]$: Crystal direction
  (hkl): Crystal plane direction
  $[hkl]$ direction is perpendicular to the (hkl) plane in the simple cubic lattice.

Basic: Wave-particle Duality

- For matters: $p = mv$, $E = \frac{1}{2}mv^2$
- For photons: $p = \frac{h\nu}{c}$, $E = h\nu$, $\nu = \frac{c}{\lambda}$
- For both: $k = \frac{2\pi}{\lambda}$, $p = \frac{h}{\lambda}$, $\hbar = \frac{h}{2\pi}$, $\Delta p \Delta x \geq \hbar$, $\Delta E \Delta t \geq \hbar$

Solution of 2nd Order DE

- $\frac{\partial^2 y}{\partial x^2} = k^2 y$

$$y = Ae^{kx} + Be^{-kx}$$

- $\frac{\partial^2 y}{\partial x^2} = -k^2 y$

$$y = Ae^{ikx} + Be^{-ikx}$$
$$= C\sin(kx) + D\cos(kx)$$

Basic Concepts

- Wave function: $\Psi(x)$
- Probability density function: $|\Psi(x)|^2 = \Psi(x)\Psi^*(x)$.
- Schrodinger Equation:

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0$$

- Boundary condition:
  - $\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$
  - $\Psi(x)$ must be finite
  - $\Psi(x)$ must be continuous
  - $\partial\Psi(x)/\partial x$ must be finite
  - $\partial\Psi(x)/\partial x$ must be continuous (when $V(x) < \infty$)

Electrons in Free Space

- Suppose $V(x) = 0$

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$$

- General solution:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

  where the wave number $k = \sqrt{\frac{2mE}{\hbar}}$.

- Particles in free space behave as traveling waves, and we have $k = \sqrt{\frac{2mE}{\hbar}} = \frac{p}{\hbar}$, $\lambda = \frac{h}{p} = \frac{2\pi}{k}$.

Electrons in Infinite Quantum Well

- $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0,$ $\begin{cases} V(x) = +\infty, & x \leq 0 \text{ or } x \geq a \\ V(x) = 0, & 0 < x < a \end{cases}$

- General solution:

$$\Psi(x) = A_1 \cos kx + A_2 \sin kx$$

- Boundary condition:

$$\Psi(x = 0) = \Psi(x = a) = 0$$

$$\int_0^a \Psi(x)\Psi^*(x) = 1$$

- Conclusion:

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin k_n x$$

$$k_n = \frac{n\pi}{a}, n = 1, 2, 3, \cdots$$

$$E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

Electrons in Finite Quantum Well

- $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0, \begin{cases} V(x) = V_0, & x \le 0 \text{ or } x \ge a \\ V(x) = 0, & 0 < x < a \end{cases}$

- General solution:

$$\Psi(x) = \begin{cases} Ae^{-ik_1 x} + Be^{ik_1 x}, & k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, x \le 0 \text{ or } x \ge a \\ Ce^{-ik_2 x} + De^{ik_2 x}, & k_2 = \sqrt{\frac{2mE}{\hbar^2}}, 0 < x < a \end{cases}$$

- Boundary condition:

$$\Psi(x)|_{x=0,a} \text{ continuous}$$

$$\Psi^{'}(x)|_{x=0,a} \text{ continuous}$$

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x) = 1$$

- Depending on the relationship between E and V_0, $\Psi(x)$ is different.

1-D Kronig-Penny Model

- Idealized model of one dimensional single crystal
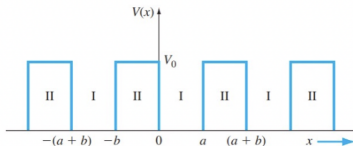
Figure: Potential function of 1-D crystal in KP model

- Bloch theorem: $\Psi(x) = u(x)e^{jkx}$
- Conclusion:

$$P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

where $P' = \frac{mV_0 ba}{\hbar^2}$. This equation gives the condition that the Schrodinger wave equation has a solution.

Energy Bands in K Space

- Consider the E-k relation of particles in the lattice.
- Let $f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$
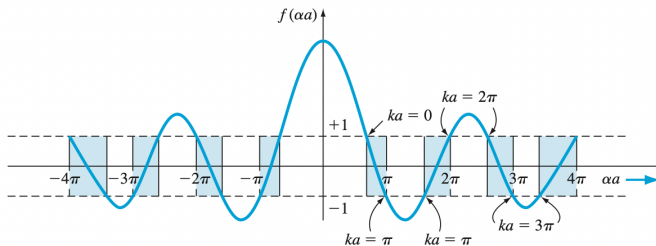
Figure: The entire $f(\alpha a)$ function

where the shared areas show the allowed values of αa corresponding to real values of k.

The E versus k diagram
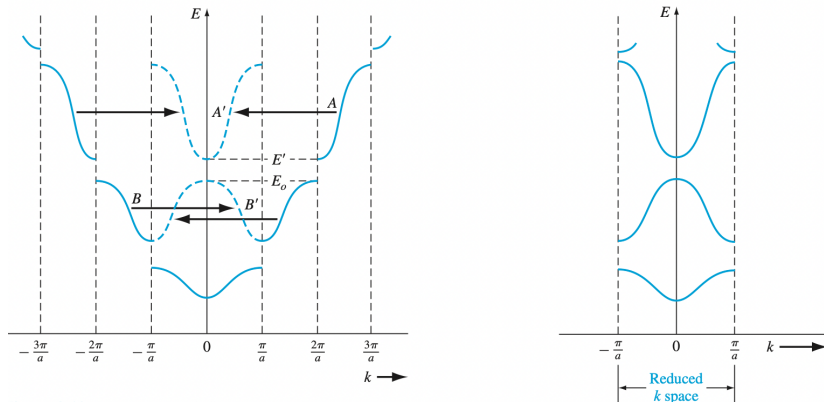
Figure: E vs. k diagram

For the same energy level, k can have 2 values. (Positive and negative direction)

Energy bands

- Semiconductor:
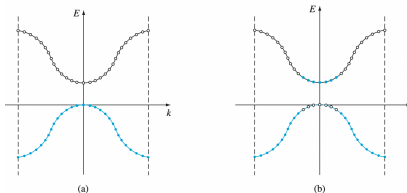
Figure: E-k diagram of semiconductor. (a)T=0K; (b)T>0K

- When external electric field is applied
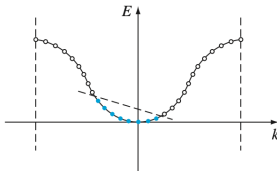
Drift current density: $J = qNv_d = q\sum_{i=1}^{N} v_i$.

Effective Mass

- Background: for the electrons in the lattice,

$$F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = ma$$

where m is the static mass of the electron. Consider only the external force,

$$F_{\text{ext}} = m^* a$$

where m^* is the effective mass of the electron.

- For electron in free space, we have $E = \frac{\hbar^2 k^2}{2m}$, i.e.,

$$\frac{1}{\hbar} \frac{dE}{dk} = v$$

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m}$$

Effective Mass

- For electrons at the bottom of the conduction band, $E - E_c = C_1(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

- For electrons at the top of the valance band, $E - E_v = -C_2(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

  which is equivalent to holes with positive mass and positive charge.

-

$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$$

$$E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$$

where m_n^* and m_p^* are effective mass of electrons and holes.

Density of States Function

- For electrons in the lattice, $E = \frac{\hbar^2 k^2}{2m}$,

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$$

- For electrons at the bottom of the conduction band, $E - E_c = \frac{\hbar^2 k^2}{2m_n^*}$,

$$g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}, \quad E \geq E_c$$

- For holes at the top of the valance band, $E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$,

$$g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}, \quad E \leq E_v$$

- There is no energy states in the forbidden band, $g(E) = 0$, when $E_v < E < E_c$.

Fermi-Dirac Probability Function

- Fermi level E_F: hypothetical levels with a 50% probability of electron occupancy in thermodynamic equilibrium.
- $f_F(E)$ represents the possibility that a quantum state of energy E is occupied by an electron

$$f_F(E) = \frac{1}{1 + \exp(\frac{E - E_F}{kT})}$$
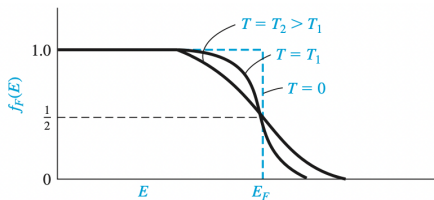
Figure: The Fermi probability function versus energy for different temperatures.

Boltzmann Distribution

- When $E - E_F > 3kT$,

$$f_F(E) \approx \exp(-\frac{E - E_F}{kT})$$

Figure: The Fermi–Dirac probability function and the Maxwell–Boltzmann approximation.

Formula

- $\frac{\partial^2 y}{\partial x^2} = k^2 y \implies y = Ae^{kx} + Be^{-kx}$

  $\frac{\partial^2 y}{\partial x^2} = -k^2 y \implies y = Ae^{ikx} + Be^{-ikx}$

- $p = mv$, $E = \frac{1}{2}mv^2$

  $p = \frac{h\nu}{c}$, $E = h\nu$, $\nu = \frac{c}{\lambda}$

  $k = \frac{2\pi}{\lambda}$, $p = \frac{h}{\lambda}$, $\hbar = \frac{h}{2\pi}$

- $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0$

- $\Psi(x) = \sqrt{\frac{2}{a}}\sin k_n x \quad k_n = \frac{n\pi}{a}, n = 1, 2, 3, \cdots, \quad E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$

- $\frac{1}{\hbar}\frac{dE}{dk} = v \quad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$

- $J = qNv_d = q\sum_{i=1}^{N} v_i$

- $E - E_c = C_1(k)^2$, $\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$

  $E - E_v = -C_2(k)^2$, $\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$

Formula

- $E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$

  $E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$

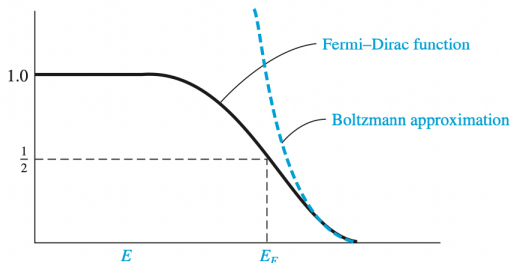- $g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$

  $g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}, \quad E \geq E_c$

  $g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}, \quad E \leq E_v$

- $f_F(E) = \frac{1}{1 + \exp(\frac{E - E_F}{kT})}$

  $f_F(E) \approx \exp(-\frac{E - E_F}{kT})$

- $n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E) dE$

  $p_0 = \int_{-\infty}^{E_v} g_v(E)(1 - f_F(E)) dE$

- $n_0 = N_c \exp\left(\frac{E_F - E_c}{kT}\right)$

  $p_0 = N_v \exp\left(\frac{E_v - E_F}{kT}\right)$

  $n_0 p_0 = N_c N_v \exp\left(-\frac{E_g}{kT}\right) = n_i^2$

Formula

- $n_0 = n_i \exp\left[\frac{E_F - E_{Fi}}{kT}\right]$

  $p_0 = n_i \exp\left[\frac{-(E_F - E_{Fi})}{kT}\right]$

- $E_{Fi} - E_{\text{midgap}} = \frac{3}{4}kT \ln\left(\frac{m_p^*}{m_n^*}\right)$

- $\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{N_c}{2N_d} \exp\left[\frac{-(E_c - E_d)}{kT}\right]}$

- $n_0 = \frac{(N_d - N_a)}{2} + \sqrt{\left(\frac{N_d - N_a}{2}\right)^2 + n_i^2}$

  $p_0 = \frac{(N_a - N_d)}{2} + \sqrt{\left(\frac{N_a - N_d}{2}\right)^2 + n_i^2}$

- $E_c - E_F = kT \ln\left(\frac{N_c}{n_0}\right)$ (when $N_d \gg n_i$, $E_c - E_F = kT \ln\left(\frac{N_c}{N_d}\right)$)

  $E_F - E_{Fi} = kT \ln\left(\frac{n_0}{n_i}\right)$

- $E_F - E_v = kT \ln\left(\frac{N_v}{p_0}\right)$ (when $N_a \gg n_i$, $E_F - E_v = kT \ln\left(\frac{N_v}{N_a}\right)$)

  $E_{Fi} - E_F = kT \ln\left(\frac{p_0}{n_i}\right)$

Formula

- $I_{drf} = e(\mu_n n + \mu_p p)E$
- $\rho = \frac{1}{\sigma} = \frac{1}{e(\mu_n n + \mu_p p)}$
- $v_n = \frac{v_s}{\left[1 + (\frac{E_{on}}{E})^2\right]^{1/2}}$
  $v_p = \frac{v_s}{\left[1 + (\frac{E_{op}}{E})^2\right]^{1/2}}$
- $J_{nx|dif} = eD_n \frac{dn}{dx}$
  $J_{px|dif} = -eD_p \frac{dp}{dx}$
- $\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{kT}{e}$

Table

Table B.2 | Conversion factors

	Prefixes		
1 Å (angstrom) = 10^{-8} cm = 10^{-10} m	10^{-15}	femto-	= f
1 μm (micrometer) = 10^{-4} cm	10^{-12}	pico-	= p
1 mil = 10^{-3} in. = 25.4 μm	10^{-9}	nano-	= n
2.54 cm = 1 in.	10^{-6}	micro-	= μ
1 eV = 1.6×10^{-19} J	10^{-3}	milli-	= m
1 J = 10^{7} erg	10^{+3}	kilo-	= k
	10^{+6}	mega-	= M
	10^{+9}	giga-	= G
	10^{+12}	tera-	= T

Table

Table B.3 | Physical constants

Avogadro's number	$N_A = 6.02 \times 10^{+23}$ atoms per gram molecular weight
Boltzmann's constant	$k = 1.38 \times 10^{-23}$ J/K $= 8.62 \times 10^{-5}$ eV/K
Electronic charge (magnitude)	$e = 1.60 \times 10^{-19}$ C
Free electron rest mass	$m_0 = 9.11 \times 10^{-31}$ kg
Permeability of free space	$\mu_0 = 4\pi \times 10^{-7}$ H/m
Permittivity of free space	$\epsilon_0 = 8.85 \times 10^{-14}$ F/cm $= 8.85 \times 10^{-12}$ F/m
Planck's constant	$h = 6.625 \times 10^{-34}$ J-s $= 4.135 \times 10^{-15}$ eV-s
	$\dfrac{h}{2\pi} = \hbar = 1.054 \times 10^{-34}$ J-s
Proton rest mass	$M = 1.67 \times 10^{-27}$ kg
Speed of light in vacuum	$c = 2.998 \times 10^{10}$ cm/s
Thermal voltage ($T = 300$ K)	$V_t = \dfrac{kT}{e} = 0.0259$ V
	$kT = 0.0259$ eV

Table

Property	Si	GaAs	Ge
Atoms (cm^{-3})	5.0×10^{22}	4.42×10^{22}	4.42×10^{22}
Atomic weight	28.09	144.63	72.60
Crystal structure	Diamond	Zincblende	Diamond
Density (g/cm^3)	2.33	5.32	5.33
Lattice constant (Å)	5.43	5.65	5.65
Melting point (°C)	1415	1238	937
Dielectric constant	11.7	13.1	16.0
Bandgap energy (eV)	1.12	1.42	0.66
Electron affinity, χ (V)	4.01	4.07	4.13
Effective density of states in conduction band, N_c (cm^{-3})	2.8×10^{19}	4.7×10^{17}	1.04×10^{19}
Effective density of states in valence band, N_v (cm^{-3})	1.04×10^{19}	7.0×10^{18}	6.0×10^{18}
Intrinsic carrier concentration (cm^{-3})	1.5×10^{10}	1.8×10^{6}	2.4×10^{13}
Mobility (cm^2/V-s)			
Electron, μ_n	1350	8500	3900
Hole, μ_p	480	400	1900
Effective mass $\left(\dfrac{m^*}{m_0}\right)$			
Electrons	$m_l^* = 0.98$ $m_t^* = 0.19$	0.067	1.64 0.082
Holes	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	0.082 0.45	0.044 0.28
Density of states effective mass			
Electrons $\left(\dfrac{m_{dn}^*}{m_o}\right)$	1.08	0.067	0.55
Holes $\left(\dfrac{m_{dp}^*}{m_o}\right)$	0.56	0.48	0.37
Conductivity effective mass			
Electrons $\left(\dfrac{m_{cn}^*}{m_o}\right)$	0.26	0.067	0.12
Holes $\left(\dfrac{m_{cp}^*}{m_o}\right)$	0.37	0.34	0.21

Table

Table B.5 | Other semiconductor parameters

Material	E_g (eV)	a (Å)	ϵ_r	χ	$\bar{n}$
Aluminum arsenide	2.16	5.66	12.0	3.5	2.97
Gallium phosphide	2.26	5.45	10	4.3	3.37
Aluminum phosphide	2.43	5.46	9.8		3.0
Indium phosphide	1.35	5.87	12.1	4.35	3.37

Table B.6 | Properties of SiO_2 and Si_3N_4 ($T = 300$ K)

Property	SiO_2	Si_3N_4
Crystal structure	[Amorphous for most integrated circuit applications]	
Atomic or molecular density (cm^{-3})	2.2×10^{22}	1.48×10^{22}
Density (g/cm^3)	2.2	3.4
Energy gap	≈ 9 eV	4.7 eV
Dielectric constant	3.9	7.5
Melting point (°C)	≈ 1700	≈ 1900

Table

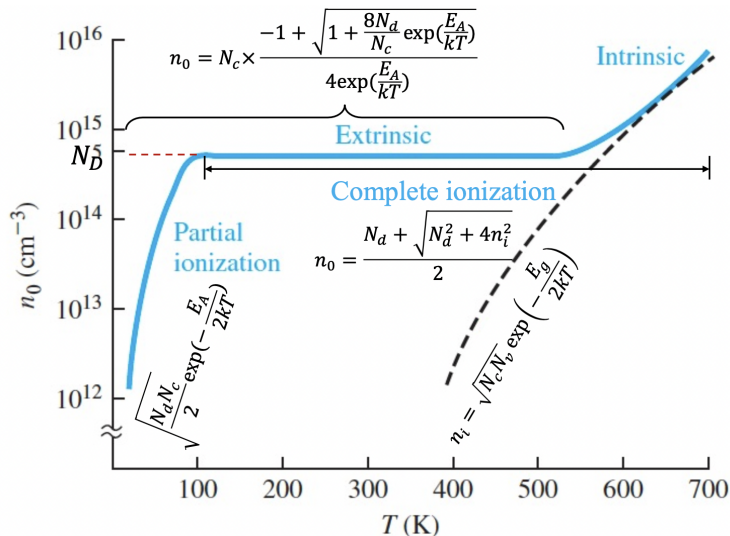**Table 4.1 |** Effective density of states function and density of states effective mass values

	N_c (cm^{-3})	N_v (cm^{-3})	m_n^*/m_0	m_p^*/m_0
Silicon	2.8×10^{19}	1.04×10^{19}	1.08	0.56
Gallium arsenide	4.7×10^{17}	7.0×10^{18}	0.067	0.48
Germanium	1.04×10^{19}	6.0×10^{18}	0.55	0.37

Table 4.2 | Commonly accepted values of n_i at $T = 300$ K

Silicon	$n_i = 1.5 \times 10^{10}$ cm^{-3}
Gallium arsenide	$n_i = 1.8 \times 10^{6}$ cm^{-3}
Germanium	$n_i = 2.4 \times 10^{13}$ cm^{-3}

Table

Good Luck!