

# VE320 Intro to Semiconductor Devices

## Mid1 Recitation Class

Ziyi Wang

UM-SJTU Joint Institute

June 10, 2022

# Contents

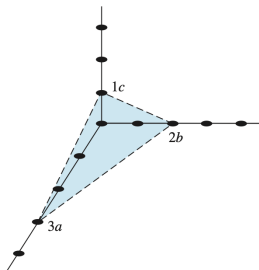
- 1 Chapter 1: Crystalline Structure of Solids
  - Space Lattice
- 2 Chapter 2: Introduction to Quantum Mechanics
  - Basic Equations
  - Schrodinger Wave Equation
- 3 Chapter 3: Quantum Theory of Solids
  - Allowed & Forbidden Energy Bands
  - Electrical Conduction in Solid
  - Density of States Function
  - Statistical Mechanics
- 4 Formulas and Tables

- 1 Chapter 1: Crystalline Structure of Solids
  - Space Lattice
- 2 Chapter 2: Introduction to Quantum Mechanics
  - Basic Equations
  - Schrodinger Wave Equation
- 3 Chapter 3: Quantum Theory of Solids
  - Allowed & Forbidden Energy Bands
  - Electrical Conduction in Solid
  - Density of States Function
  - Statistical Mechanics
- 4 Formulas and Tables

# Lattice Types

- Simple cubic:  $\#atom = \frac{1}{8} \times 8 = 1$ ,  $r(atom) = \frac{a}{2}$
- Body-centered cubic:  $\#atom = \frac{1}{8} \times 8 + 1 = 2$ ,  $r(atom) = \frac{\sqrt{3}a}{4}$
- Face-centered cubic:  $\#atom = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$ ,  $r(atom) = \frac{\sqrt{2}a}{4}$
- Volume Density =  $\frac{\#atoms \text{ per unit cell}}{\text{volume of unit cell}}$
- Surface Density =  $\frac{\#atoms \text{ per lattice plane}}{\text{area of lattice plane}}$
- 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 ( $\infty$  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.

- 1 Chapter 1: Crystalline Structure of Solids
  - Space Lattice
- 2 Chapter 2: Introduction to Quantum Mechanics
  - Basic Equations
  - Schrodinger Wave Equation
- 3 Chapter 3: Quantum Theory of Solids
  - Allowed & Forbidden Energy Bands
  - Electrical Conduction in Solid
  - Density of States Function
  - Statistical Mechanics
- 4 Formulas and Tables

# Basic: Wave-particle Duality

- For matters:  $p = mv$ ,  $E = \frac{1}{2}mv^2$
- For photons:  $p = \frac{h\nu}{c}$ ,  $E = h\nu$ ,  $\nu = \frac{\lambda}{c}$
- 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

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

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

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

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



# Basic Concepts

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

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

- 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

$$k = \sqrt{\frac{2mE}{\hbar}} = \frac{p}{\hbar}, \quad \lambda = \frac{h}{p} = \frac{2\pi}{k}.$$

# 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:

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

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

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

# Electrons in Finite Quantum Well

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

- General solution:

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

- 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 Chapter 1: Crystalline Structure of Solids

- Space Lattice

## 2 Chapter 2: Introduction to Quantum Mechanics

- Basic Equations
- Schrodinger Wave Equation

## 3 Chapter 3: Quantum Theory of Solids

- Allowed & Forbidden Energy Bands
- Electrical Conduction in Solid
- Density of States Function
- Statistical Mechanics

## 4 Formulas and Tables

# 1-D Kronig-Penny Model

- Idealized model of one dimensional single crystal

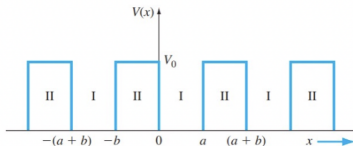


Figure: Potential function of 1-D crystal in KP model

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

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

where  $P' = \frac{mV_0ba}{\hbar^2}$ . 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  $f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$

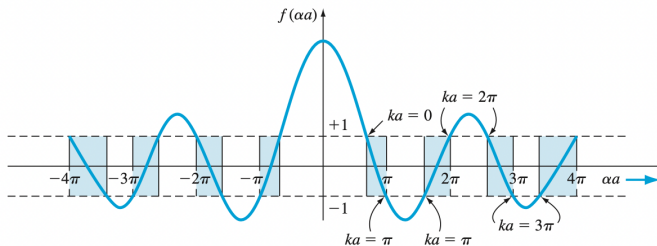


Figure: The entire  $f(\alpha a)$  function

where the shaded areas show the allowed values of  $\alpha a$  corresponding to real values of  $k$ .

# The E versus k diagram

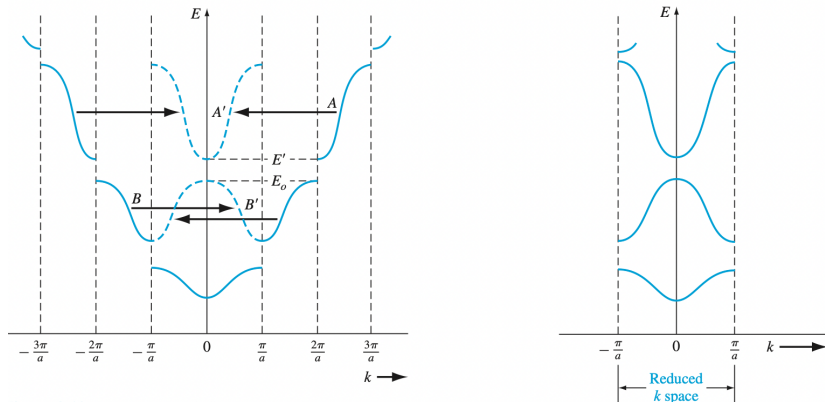


Figure: E vs. k diagram

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



# Energy bands

- Semiconductor:

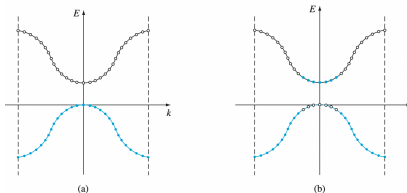
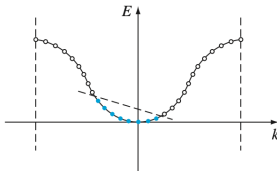


Figure: E-k diagram of semiconductor. (a) T=0K; (b) T>0K

- 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.,

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

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

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

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,  $E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$ ,

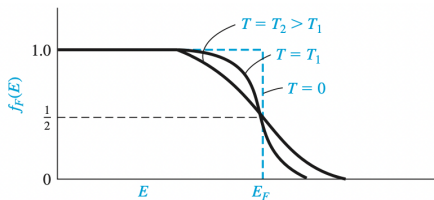
$$g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E}, \quad E \leq E_v$$

- 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

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

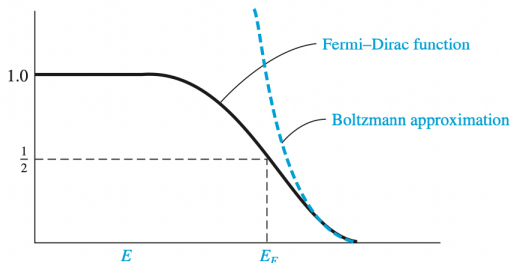


**Figure:** The Fermi probability function versus energy for different temperatures.

# Boltzmann Distribution

- When  $E - E_F > 3kT$ ,

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



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

- 1 Chapter 1: Crystalline Structure of Solids
  - Space Lattice
- 2 Chapter 2: Introduction to Quantum Mechanics
  - Basic Equations
  - Schrodinger Wave Equation
- 3 Chapter 3: Quantum Theory of Solids
  - Allowed & Forbidden Energy Bands
  - Electrical Conduction in Solid
  - Density of States Function
  - Statistical Mechanics
- 4 **Formulas and Tables**

# Formula

- $\frac{\partial^2 y}{\partial x^2} = k^2 y \implies y = Ae^{kx} + Be^{-kx}$   
 $\frac{\partial^2 y}{\partial x^2} = -k^2 y \implies y = Ae^{ikx} + Be^{-ikx}$
- $p = mv, E = \frac{1}{2}mv^2$   
 $p = \frac{h\nu}{c}, E = h\nu, \nu = \frac{\lambda}{c}$   
 $k = \frac{2\pi}{\lambda}, p = \frac{h}{\lambda}, \hbar = \frac{h}{2\pi}$
- $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar}(E - V(x))\Psi(x) = 0$
- $\Psi(x) = \sqrt{\frac{2}{a}} \sin k_n x \quad k_n = \frac{n\pi}{a}, n = 1, 2, 3, \dots, \quad E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$
- $\frac{1}{\hbar} \frac{dE}{dk} = v \quad \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m}$
- $J = qNv_d = q \sum_{i=1}^N v_i$
- $E - E_c = C_1(k)^2, \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$   
 $E - E_v = -C_2(k)^2, \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$



# Formula

- $E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$   
 $E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$
- $g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{E}$   
 $g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c}, \quad E \geq E_c$   
 $g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E}, \quad E \leq E_v$
- $f_F(E) = \frac{1}{1 + \exp(\frac{E - E_F}{kT})}$   
 $f_F(E) \approx \exp(-\frac{E - E_F}{kT})$
- $n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E) dE$   
 $p_0 = \int_{-\infty}^{E_v} g_v(E) (1 - f_F(E)) dE$
- $n_0 = N_c \exp(\frac{E_F - E_c}{kT})$   
 $p_0 = N_v \exp(\frac{E_v - E_F}{kT})$   
 $n_0 p_0 = N_c N_v \exp(-\frac{E_g}{kT}) = n_i^2$

# Formula

- $$n_0 = n_i \exp \left[ \frac{E_F - E_{Fi}}{kT} \right]$$
$$p_0 = n_i \exp \left[ \frac{-(E_F - E_{Fi})}{kT} \right]$$
- $$E_{Fi} - E_{\text{midgap}} = \frac{3}{4} kT \ln \left( \frac{m_p^*}{m_n^*} \right)$$
- $$\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{N_c}{2N_d} \exp \left[ \frac{-(E_c - E_d)}{kT} \right]}$$
- $$n_0 = \frac{(N_d - N_a)}{2} + \sqrt{\left( \frac{N_d - N_a}{2} \right)^2 + n_i^2}$$
$$p_0 = \frac{(N_a - N_d)}{2} + \sqrt{\left( \frac{N_a - N_d}{2} \right)^2 + n_i^2}$$
- $$E_c - E_F = kT \ln \left( \frac{N_c}{n_0} \right) \text{ (when } N_d \gg n_i, E_c - E_F = kT \ln \left( \frac{N_c}{N_d} \right))$$
$$E_F - E_{Fi} = kT \ln \left( \frac{n_0}{n_i} \right)$$
- $$E_F - E_v = kT \ln \left( \frac{N_v}{p_0} \right) \text{ (when } N_a \gg n_i, E_F - E_v = kT \ln \left( \frac{N_v}{N_a} \right))$$
$$E_{Fi} - E_F = kT \ln \left( \frac{p_0}{n_i} \right)$$

# Formula

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

# Table

**Table B.2** | Conversion factors

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

**Table B.3** | Physical constants

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

Table B.4 | Silicon, gallium arsenide, and germanium properties ( $T = 300\text{ K}$ )

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

**Table B.5** | Other semiconductor parameters

Material	$E_g$ (eV)	$a$ (Å)	$\epsilon_r$	$\chi$	$\bar{n}$
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  $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  ( $T = 300$  K)

Property	$\text{SiO}_2$	$\text{Si}_3\text{N}_4$
Crystal structure	[Amorphous for most integrated circuit applications]	
Atomic or molecular density ( $\text{cm}^{-3}$ )	$2.2 \times 10^{22}$	$1.48 \times 10^{22}$
Density ( $\text{g/cm}^3$ )	2.2	3.4
Energy gap	$\approx 9$ eV	4.7 eV
Dielectric constant	3.9	7.5
Melting point ( $^\circ\text{C}$ )	$\approx 1700$	$\approx 1900$

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

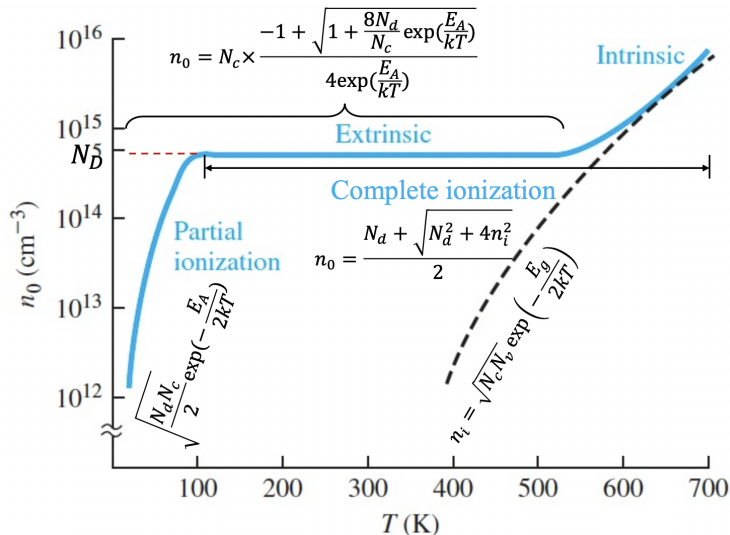
	$N_c \text{ (cm}^{-3}\text{)}$	$N_v \text{ (cm}^{-3}\text{)}$	$m_n^*/m_0$	$m_p^*/m_0$
Silicon	$2.8 \times 10^{19}$	$1.04 \times 10^{19}$	1.08	0.56
Gallium arsenide	$4.7 \times 10^{17}$	$7.0 \times 10^{18}$	0.067	0.48
Germanium	$1.04 \times 10^{19}$	$6.0 \times 10^{18}$	0.55	0.37

**Table 4.2** | Commonly accepted values of  $n_i$  at  $T = 300 \text{ K}$

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



# Table



Good Luck!

