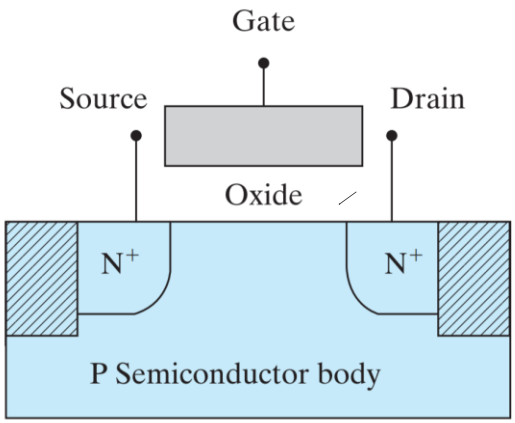
Semiconductor fundamentals_A

References:

- (C. Hu) Chapter 1
- (R. Pierret) Chapter 1



EE302

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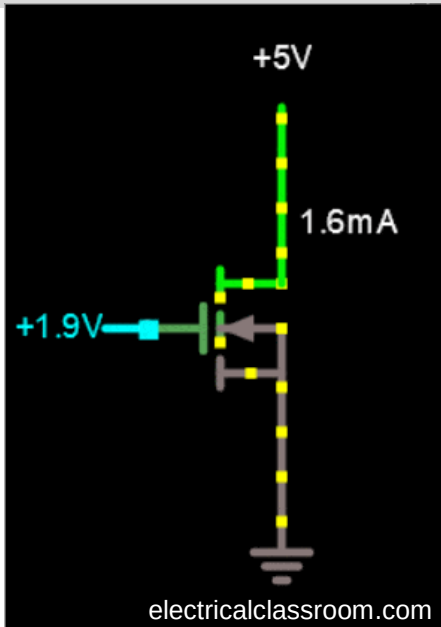
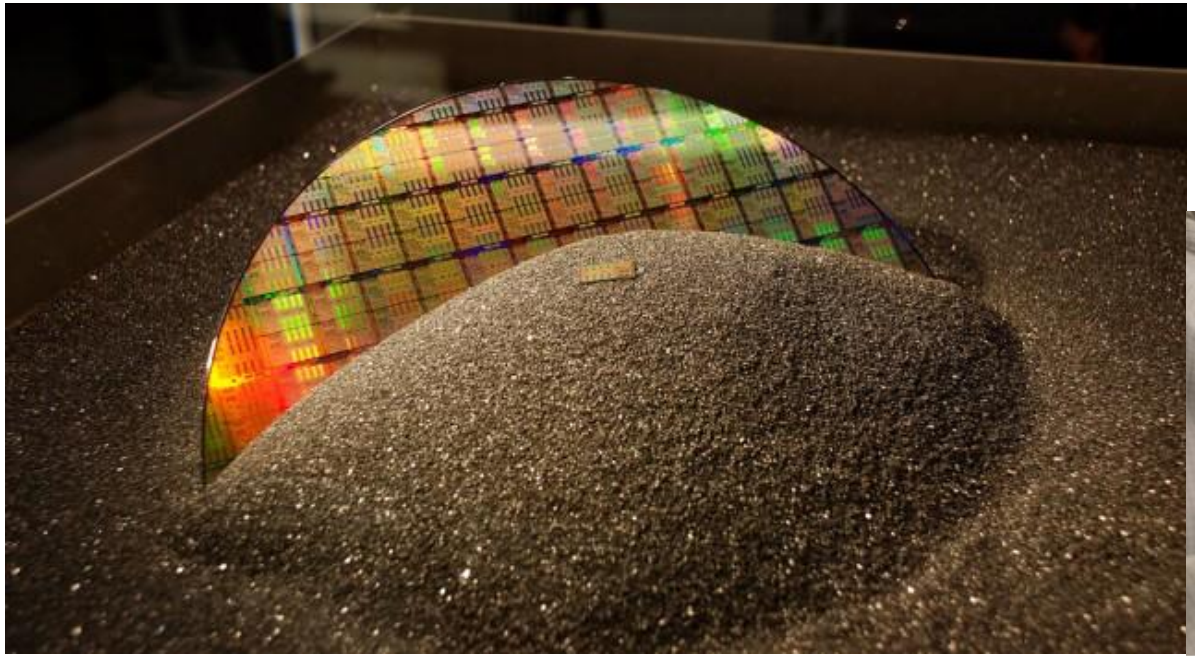
Fall 2023



Semiconductor, wafer, devices

https://asia.nikkei.com/



https://www.extremetech.com/computing/242699-450mm-silicon-wafers-arent-happening-time-soon-major-consortium-collapses

https://www.shutterstock.com/es/image-photo/technician-clean-white-suits-showing-wafer-709404757

Compositions of semiconductors

Table 1.1 Semiconductor Materials.

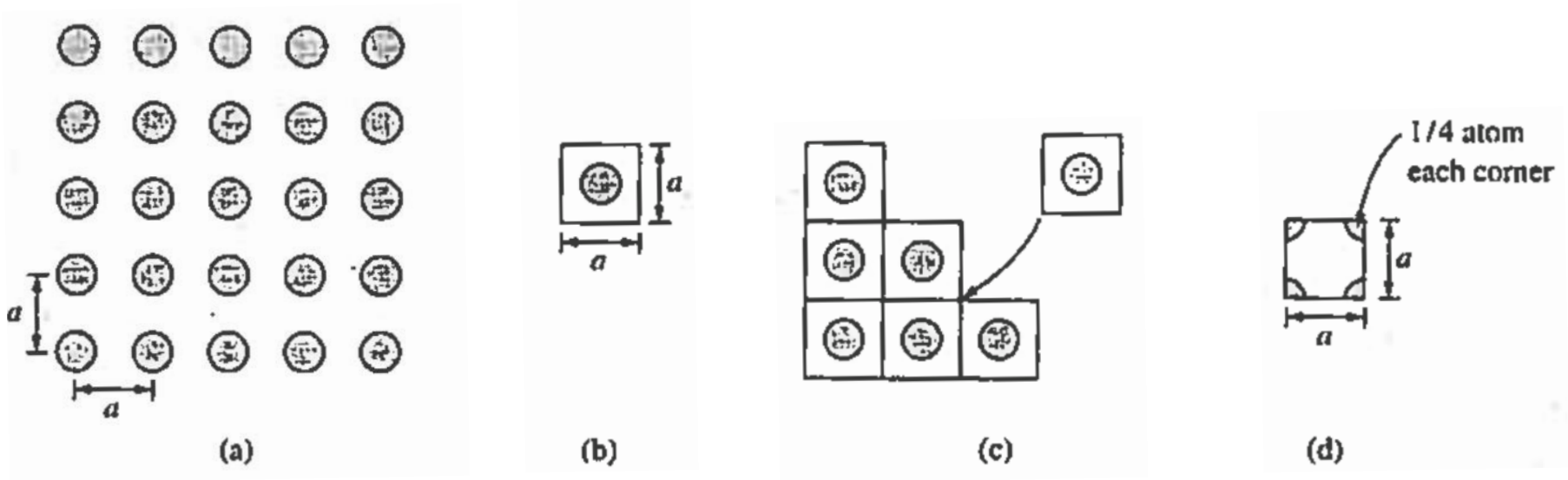
General Classification	*Semiconductor Symbol*	*Semiconductor Name*
(1) Elemental	Si	Silicon
	Ge	Germanium
(2) Compounds		
(a) IV-IV	SiC	Silicon carbide
(b) III-V	AlP	Aluminum phosphide
	AlAs	Aluminum arsenide
	AlSb	Aluminum antimonide
	GaN	Gallium nitride
	GaP	Gallium phosphide
	GaAs	Gallium arsenide
	GaSb	Gallium antimonide
	InP	Indium phosphide
	InAs	Indium arsenide
	InSb	Indium antimonide
(c) II-VI	ZnO	Zinc oxide
	ZnS	Zinc sulfide
	ZnSe	Zinc selenide
	ZnTe	Zinc telluride
	CdS	Cadmium sulfide
	CdSe	Cadmium selenide
	CdTe	Cadmium telluride
	HgS	Mercury sulfide
(d) IV-VI	PbS	Lead sulfide
	PbSe	Lead selenide
	PbTe	Lead telluride

Table 1.2 Abbreviated Periodic Chart of the Elements.

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

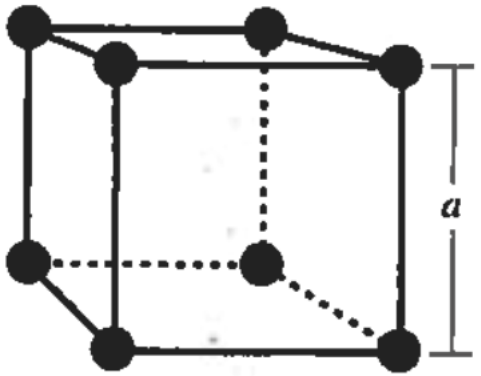
- **IV – Si, Ge**
- **III-V – GaAs, GaN, InP etc.**
- **Electrical, Optical characteristics**

Unit cell of semiconductors

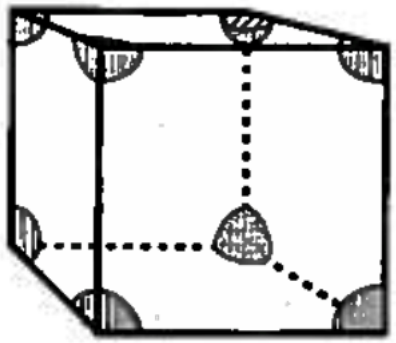


- **Most of the semiconductor material has periodicities**
- **Unit cell: reproducible to form (and represent) perfect crystal structure**
- **Can (b) and (d) both be the unit cell for (a)?**

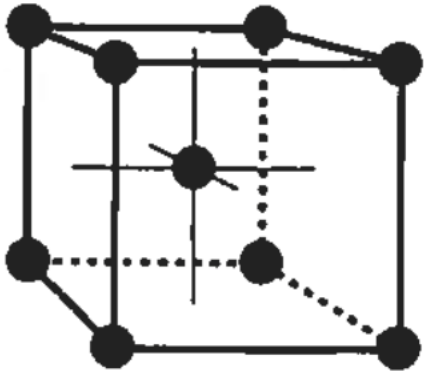
Simple 3-D unit cells



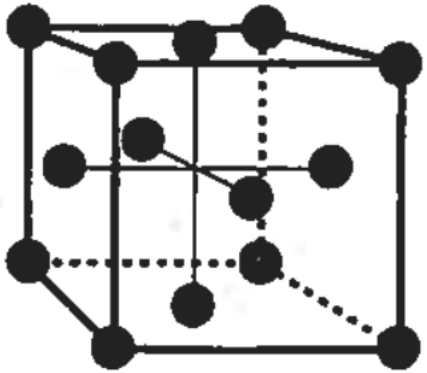
(a) Simple cubic



(b) Pedantically correct simple cubic

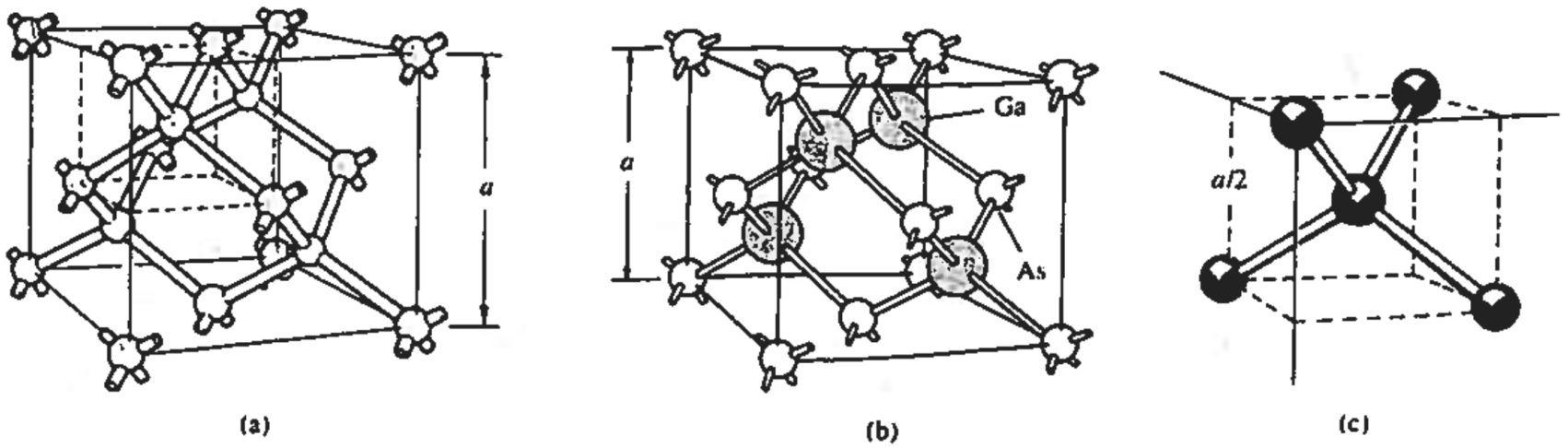


(c) bcc



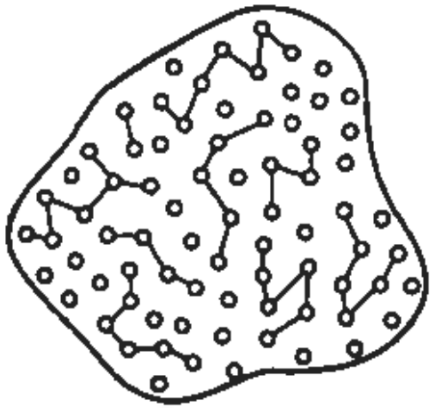
(d) fcc

- **bcc (body centered cubic unit cell); fcc (face centered cubic unit cell)**
- ***How many atoms per unit cells?***



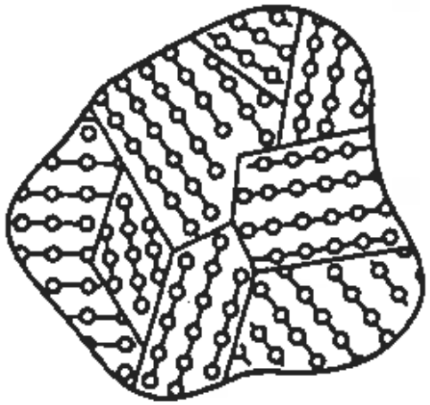
- **Si, Ge, group IV, has the unit cell structure, *diamond lattice*, in (a).**
  - ***How many atoms per cell?***
- **GaAs (III–V) has the unit cell structure, *zincblende*, in (b).**
- **Unit cell side length (a) for Si is 5.43 Å (1Å = 0.1 nm = 10^{-8} cm)**
  - ***How is this size like comapred to Modern Devices?***
- **5 x 10^{22} atoms/cm^3 for crystalline Si lattice**
- **Each atom has *FOUR* nearest neighbor atoms (c)**

Amorphous, polycrystalline, crystalline



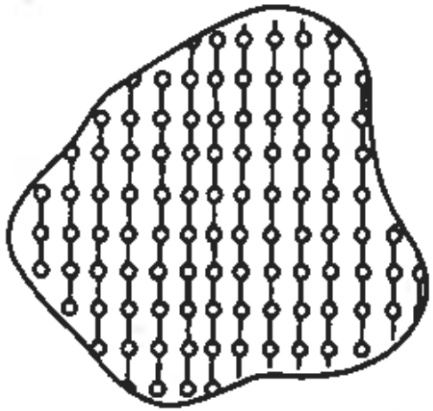
(a) Amorphous

No recognizable long-range order



(b) Polycrystalline

Completely ordered in segments

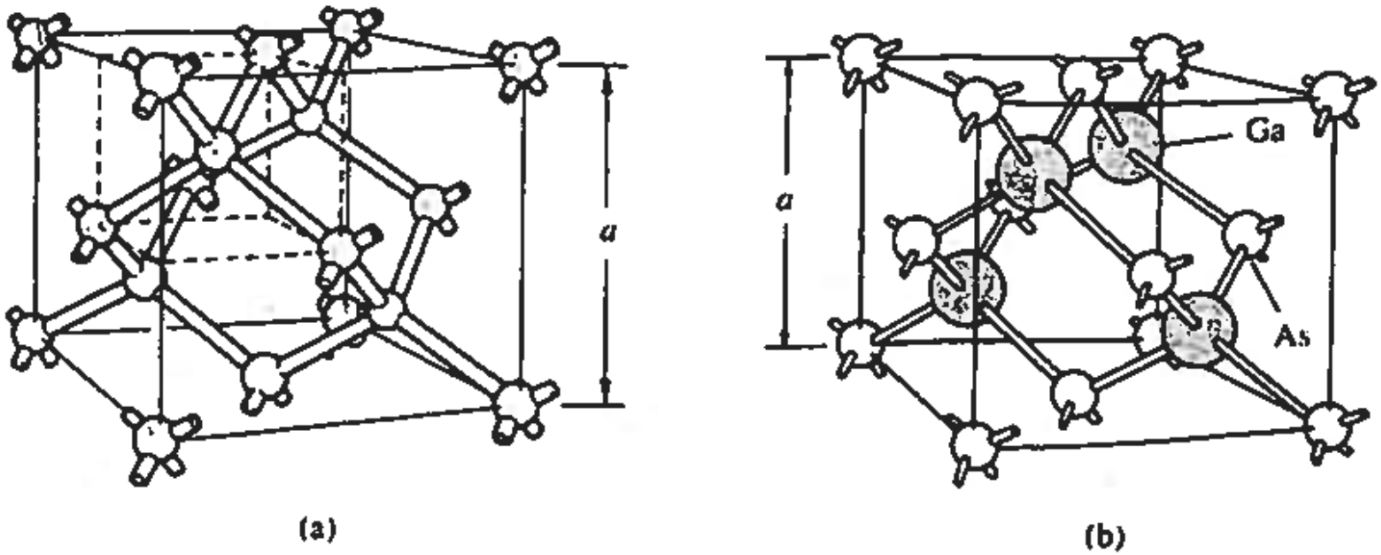


(c) Crystalline

Entire solid is made up of atoms in an orderly array

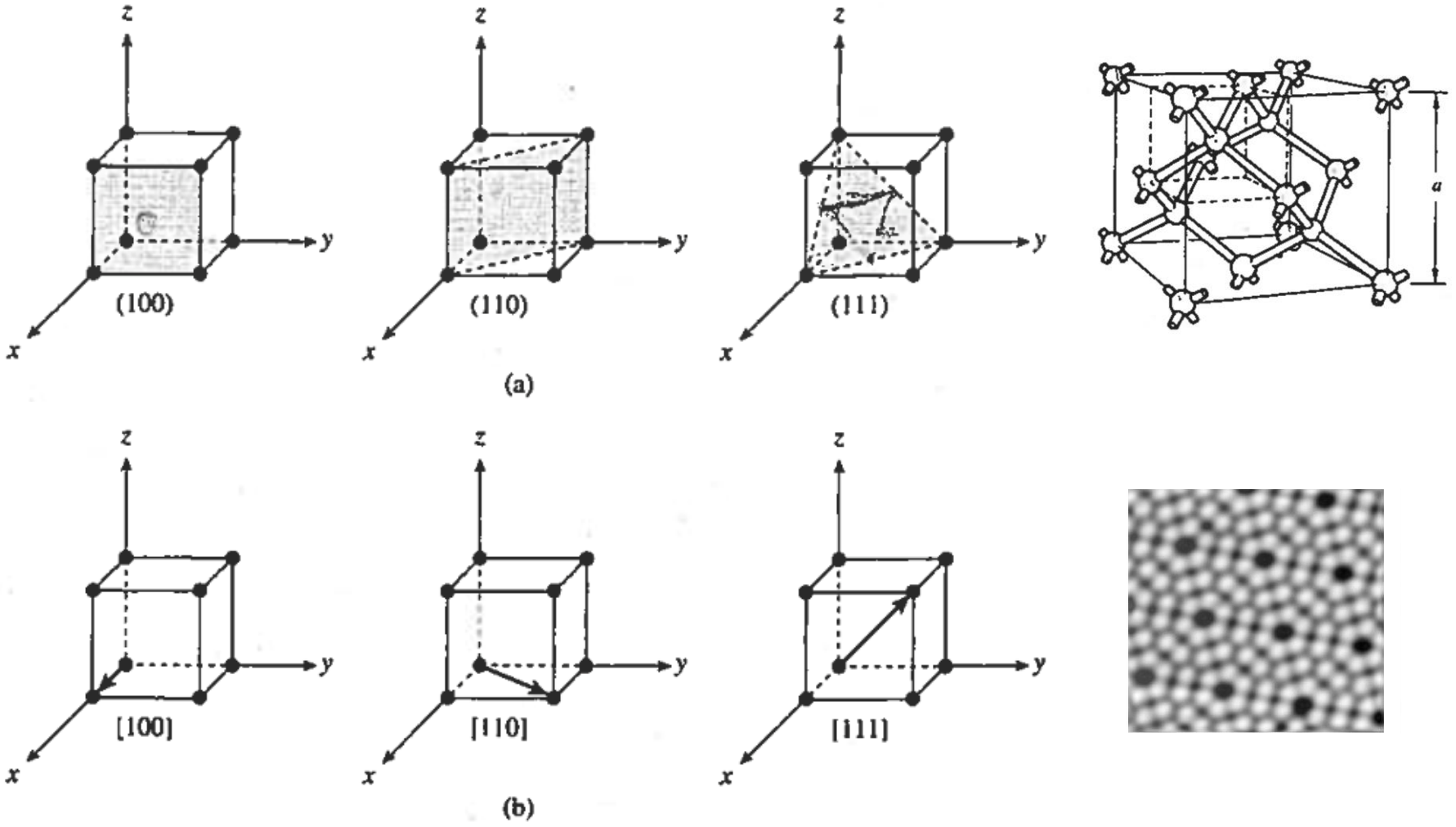
- **Different electrical characteristics**
- **Different fabrication process conditions**
- **Different applications**
- **Ideal semiconductor: in *crystalline* structure**

Purity



- **Recall: 5 x 10^{22} atoms/cm^3 for crystalline Si lattice**
- **Unintentional impurity (intrinsic): one out of 10^9 atoms (10억)**
- **Intentional impurity (dopants): one out of 10^3 ~10^8 atoms**

Miller indices



- **# of Si atoms and bonding angles are different. (*Why matters?*)**

Miller indices

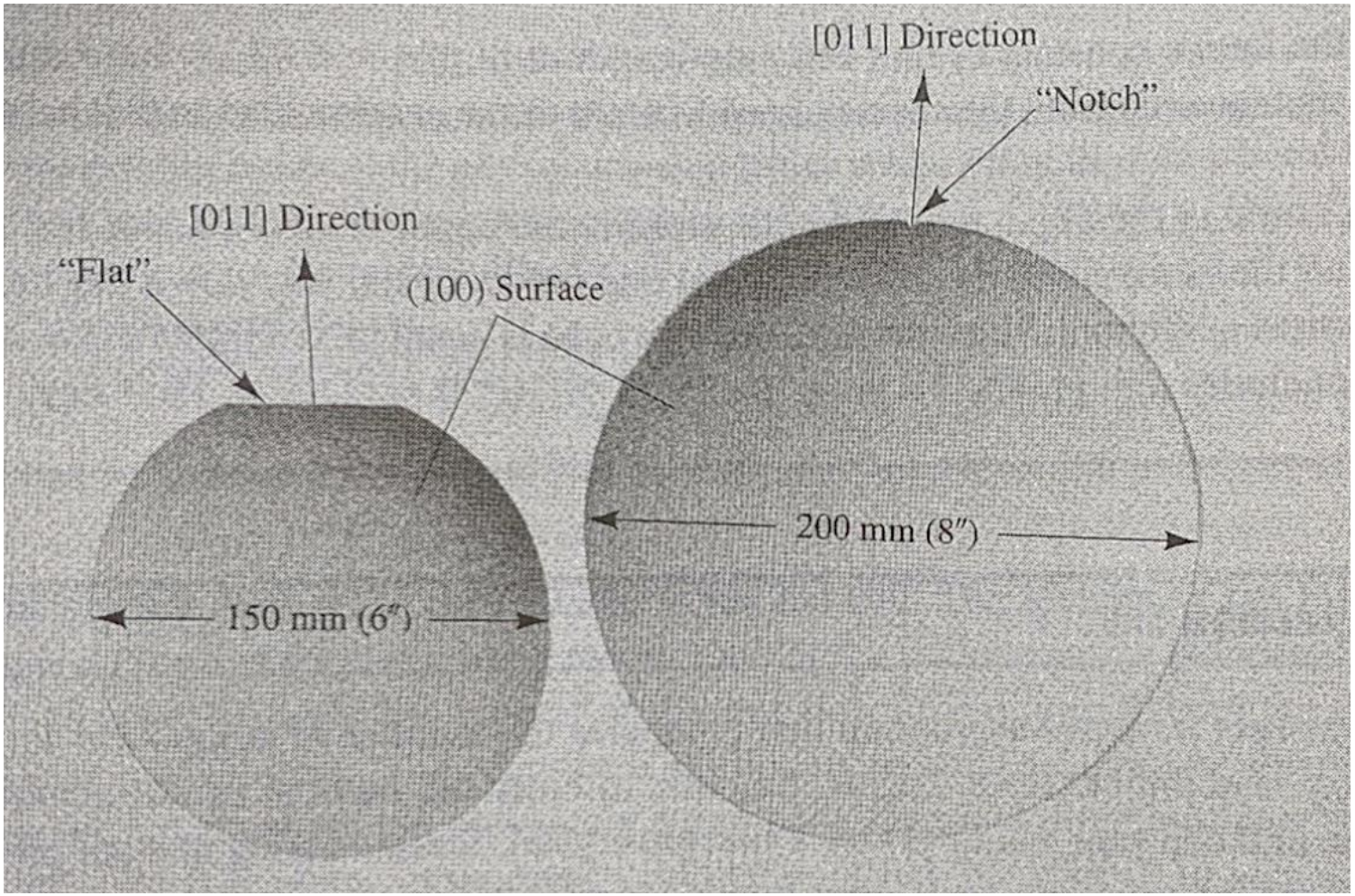
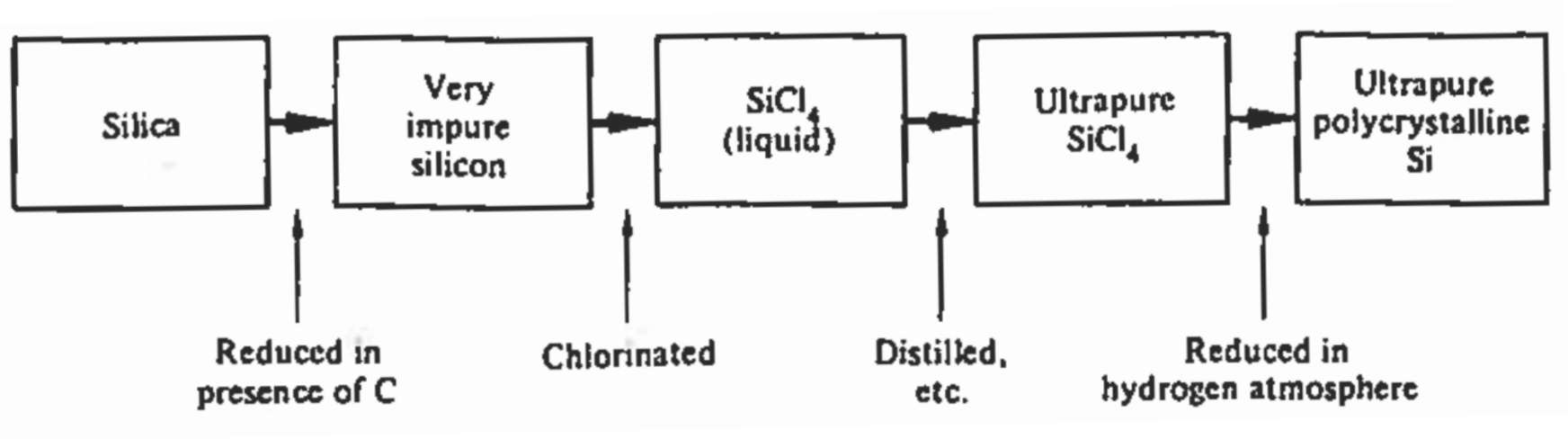


Figure 1.5 Single-crystal silicon wafers typical of the starting substrates presently employed by major device manufacturers. The 150 mm (6 inch) and 200 mm (8 inch) wafers are nominally 0.625 mm and 0.725 mm thick, respectively. The facing surface is polished and etched yielding a damage-free, mirror-like finish. The figure dramatizes the utility of Miller indices exemplified by the (100) plane and [011] direction designations. (Photograph courtesy of Intel Corporation.)

Obtaining ultrapure Si



- **Si – the 2nd most abundant element in the earth crust (the 1st?)**
  - **Silica (impure SiO_2), silicates (Si + O + another element)**
- **$SiCl_4 + 2H_2 \rightarrow 4HCl + Si$**
- **The ultrapure Si is *polycrystalline.***

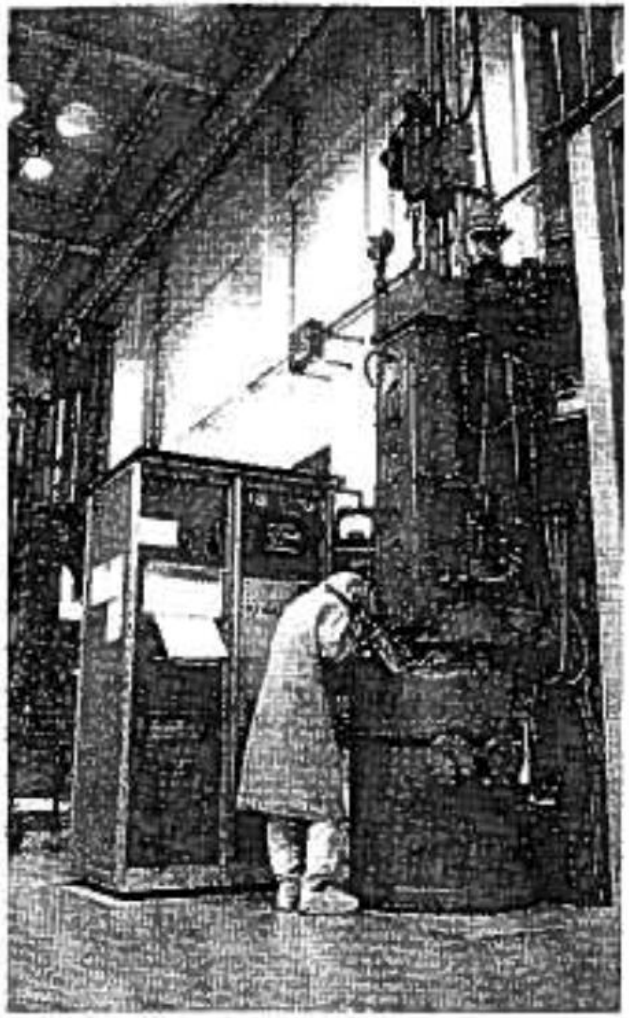
Abundance in the earth crust

Rank	Element	Atomic Number	Crustal Abundance %
1	oxygen	8	46.60
2	silicon	14	27.70
3	aluminium	13	8.13
4	iron	26	5.00
5	calcium	20	3.63
6	sodium	11	2.83
7	magnesium	12	2.59
8	potassium	19	2.09
9	titanium	22	0.44
10	hydrogen	1	0.14
10 +	Other		0.85

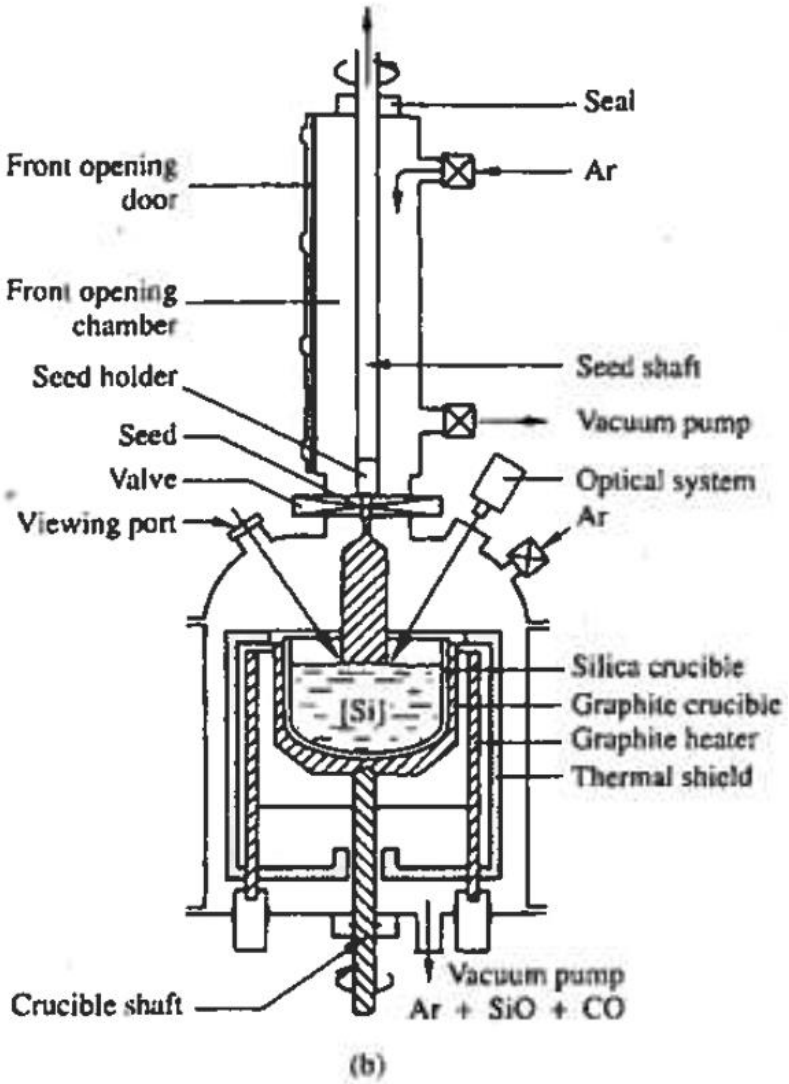
https://www.quora.com/What-are-the-ten-most-abundant-elements-in-the-earths-crust-and-their-properties

Single-crystal formation

- **Czochralski (CZ) method**



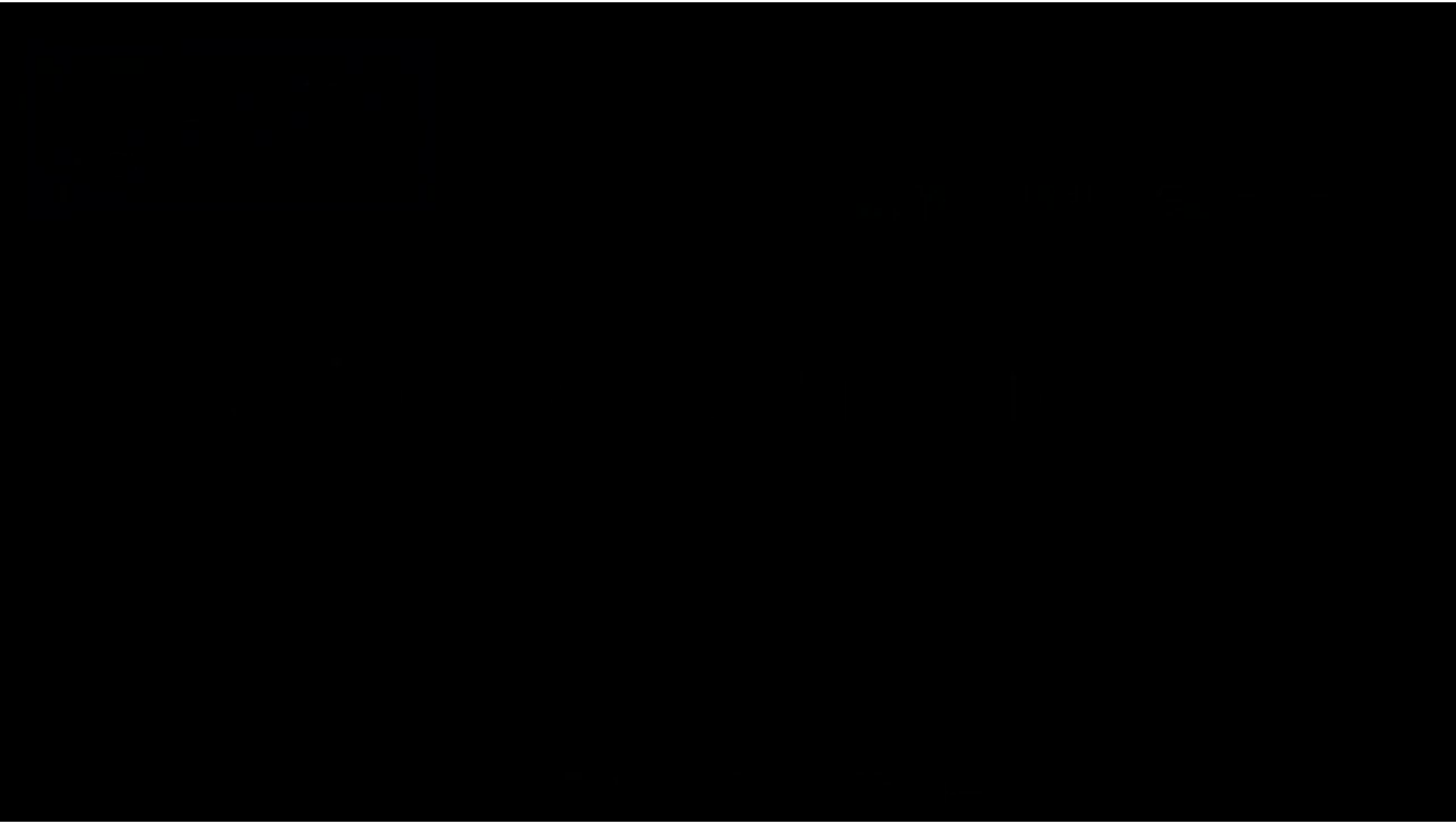
(a)



(b)

Single-crystal formation

- **Czochralski (CZ) method**



Summary

- **Group IV elements (Si, Ge), which has *four* valence electrons per atom, form diamond lattice.**
- **Single crystalline structure can perform the best as the ideal semiconductor.**
- **Single crystals of ultrapurity Si wafer is the start of everything in microelectronics.**

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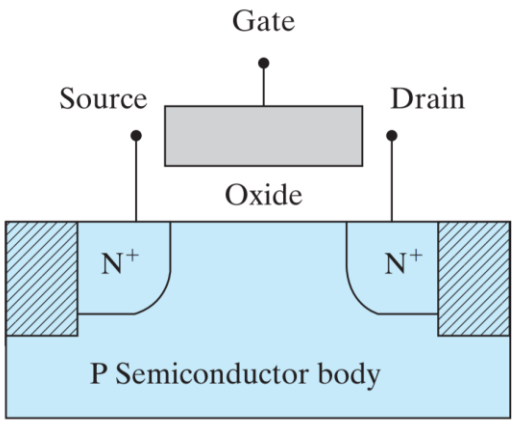
Electrons and Holes in Semiconductors (Carrier Modeling)

References:

- (C. Hu) Chapter 1
- (R. Pierret) Chapter 2



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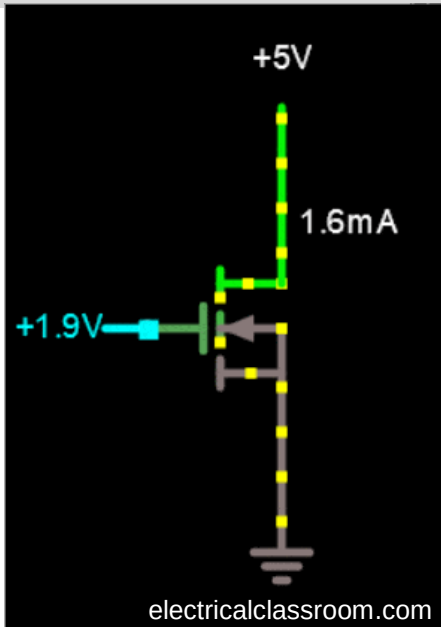
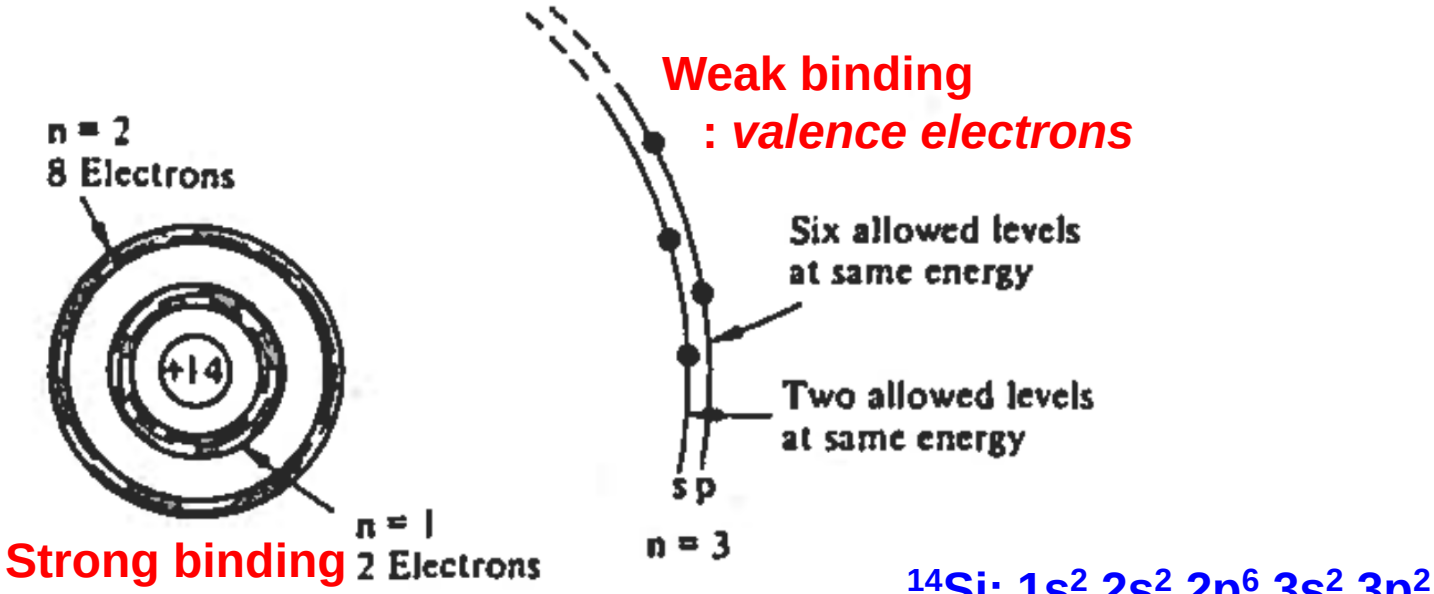


Overview

- **Main functions of Electronic Devices**
- **Carriers?**
  - **In electronic devices?**
  - **Batteries?**
  - **Metallic wires?**
- **Electrons, Holes**
- **Carrier related concepts, models, properties, terminology**
- **Why would we be interested in?**
- ***Equilibrium***
  - **“Unperturbed state of a system”**
  - **The most common perturbation in electronic devices would be…?**
  - **Invarient over time – ‘rest’ condition**

Quantization concept (atom model)

- **Bohr's atom model**
  - **Quantization of electrons' angular momentum**
  - **Quantization of available energy levels**



$^{14}Si: 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

Figure 2.2 Schematic representation of an isolated Si atom.

Bonding Model

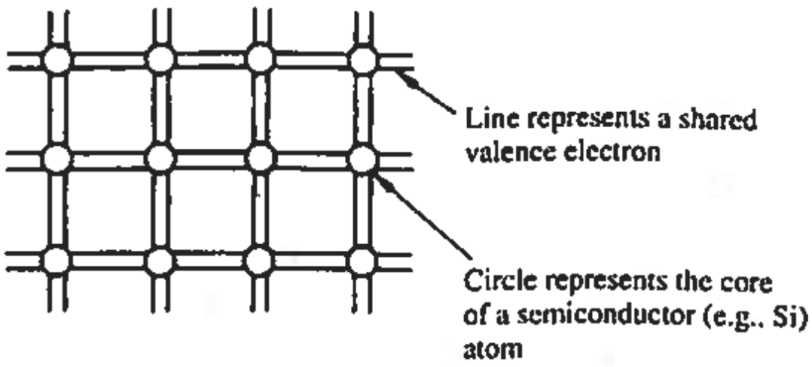
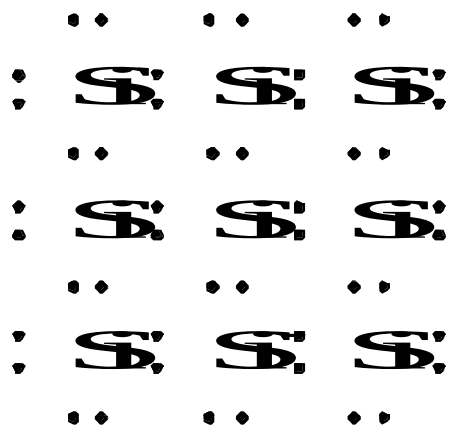


Figure 2.3 The bonding model.



- **Covalent bonding**
- ***Does it say anything about energy level?***
- ***Why would we care about energy level?***

Bonding Model

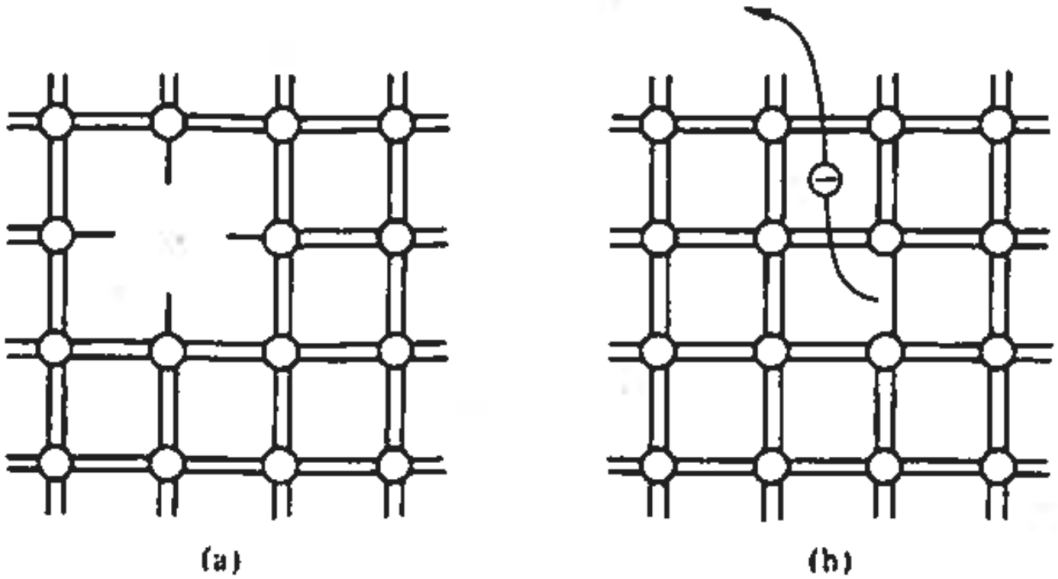
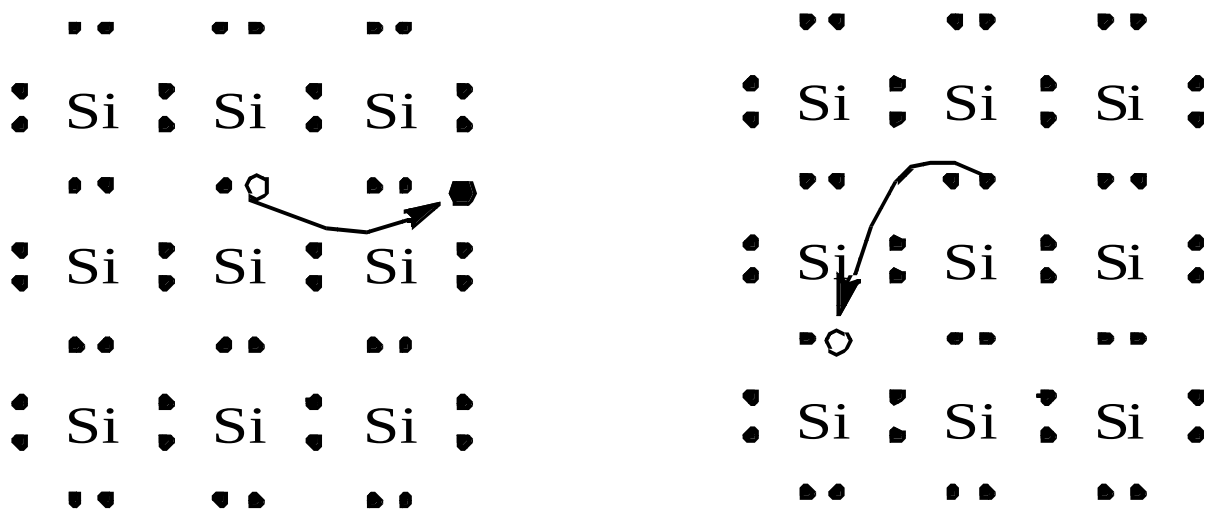


Figure 2.4 Sample utilization of the bonding model. (a) Visualization of a missing atom or point defect. (b) Breaking of an atom-to-atom bond and freeing of an electron.

- **Covalent bonding**

Bonding Model



- **Covalent bonding**

Energy Band Model

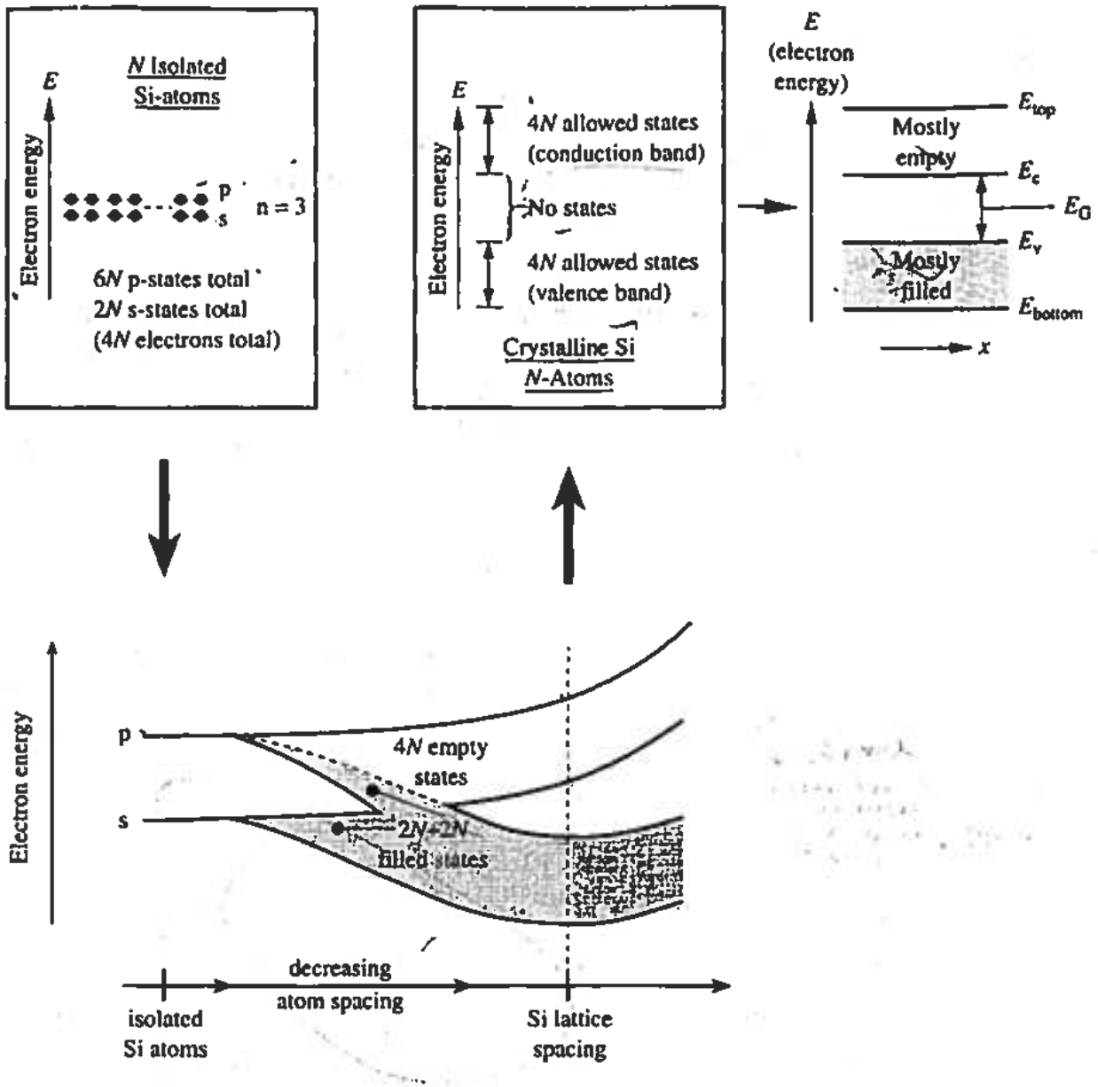
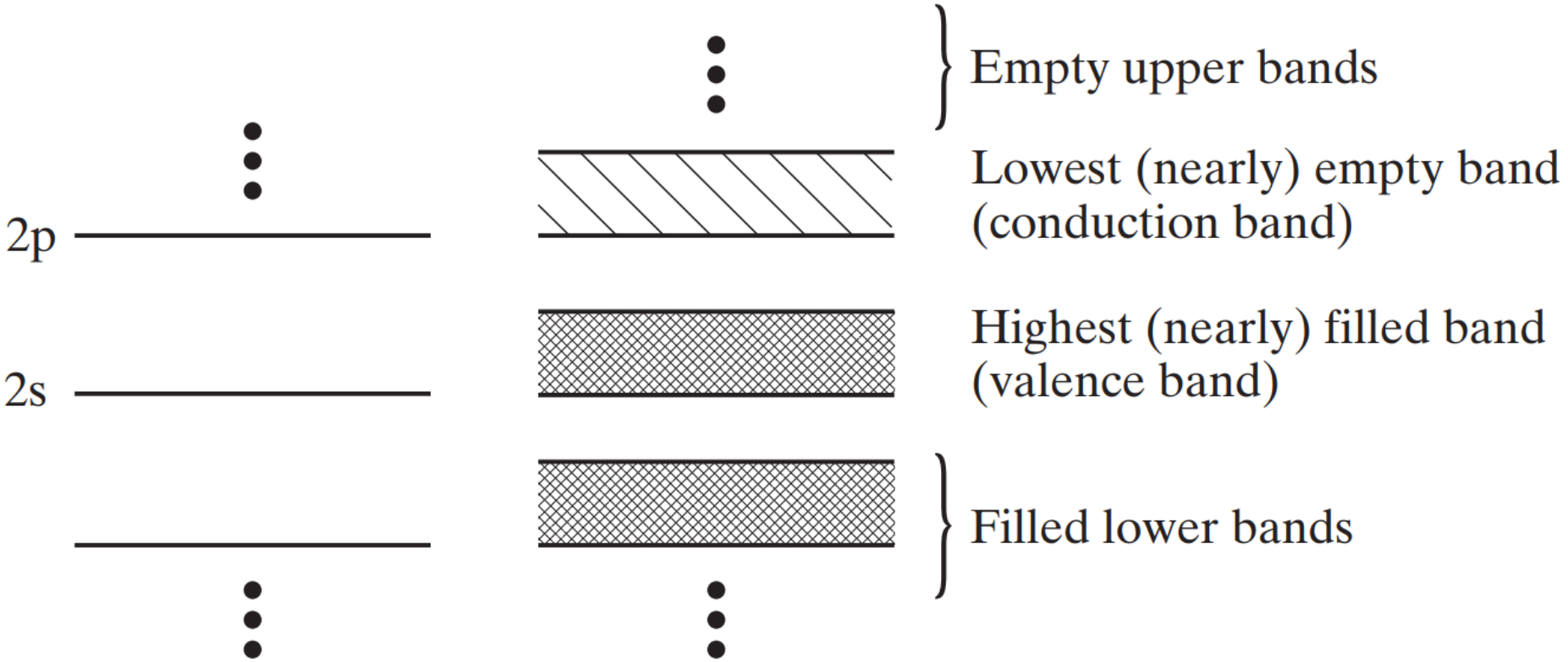


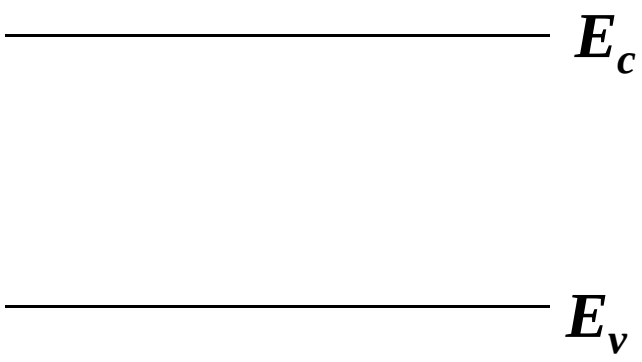
Figure 2.5 Conceptual development of the energy band model starting with N isolated Si atoms on the top left and concluding with a "dressed-up" version of the energy band model on the top right.

- **The Pauli exclusion principle**

Energy band model

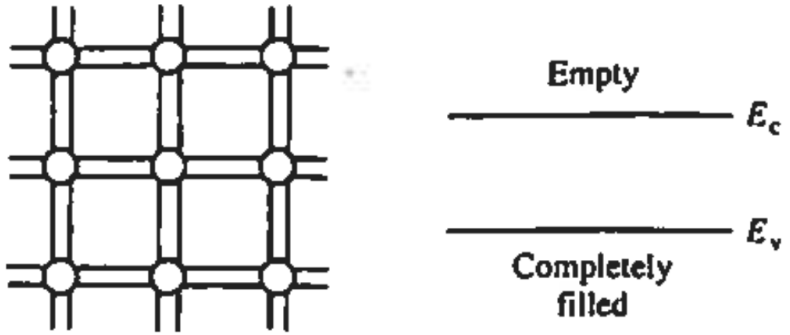


Energy band model

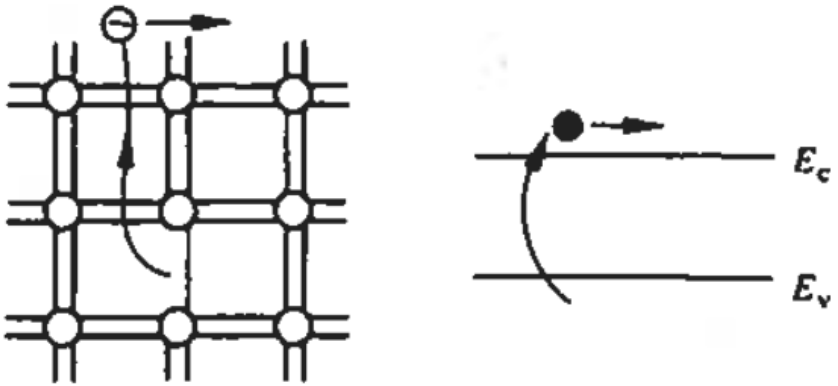


- E_c **–** Conduction band (edge)
- E_v **–** Valence band (edge)
- **Which is higher energy?**
- **In the perspective of what?**

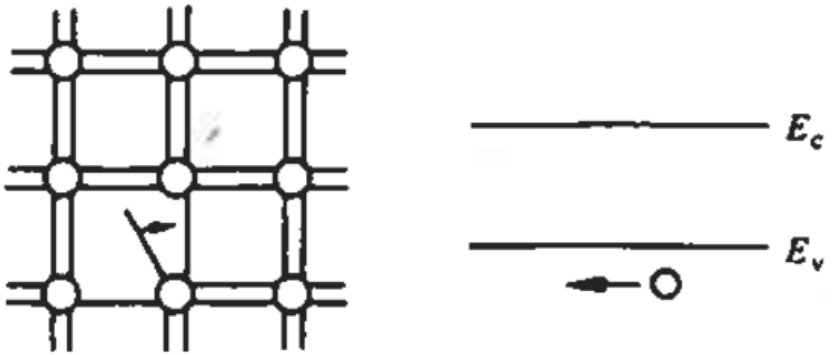
Carriers



(a) No carriers

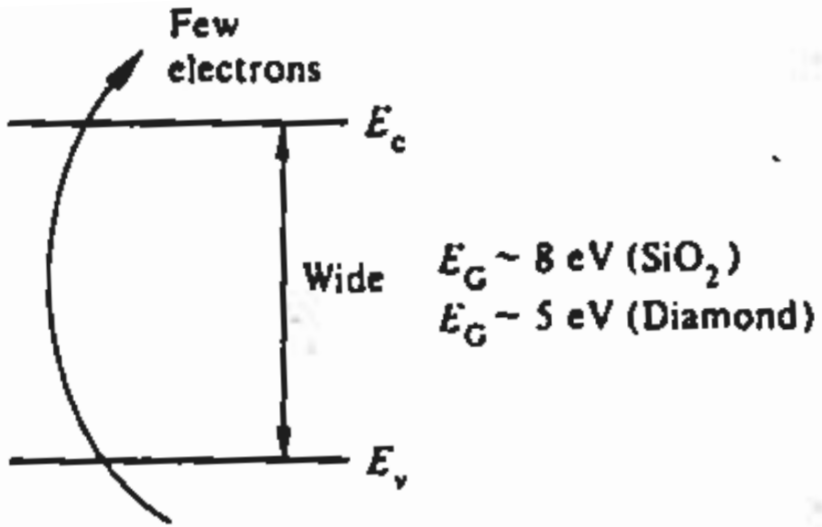


(b) The electron

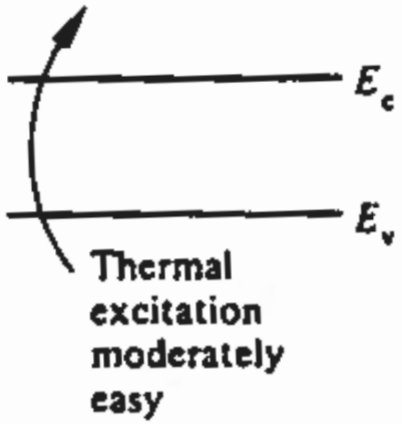


(c) The hole

Band Gap and Material Classification

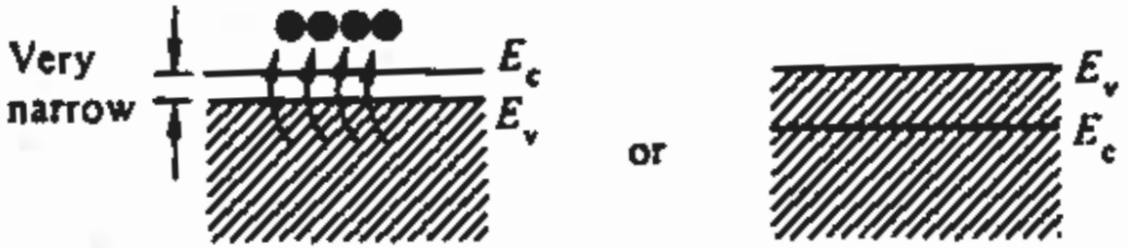


(a) Insulator



$E_G = 1.42$ eV (GaAs)
$E_G = 1.12$ eV (Si)
$E_G = 0.66$ eV (Ge)
(Room temperature)

(b) Semiconductor



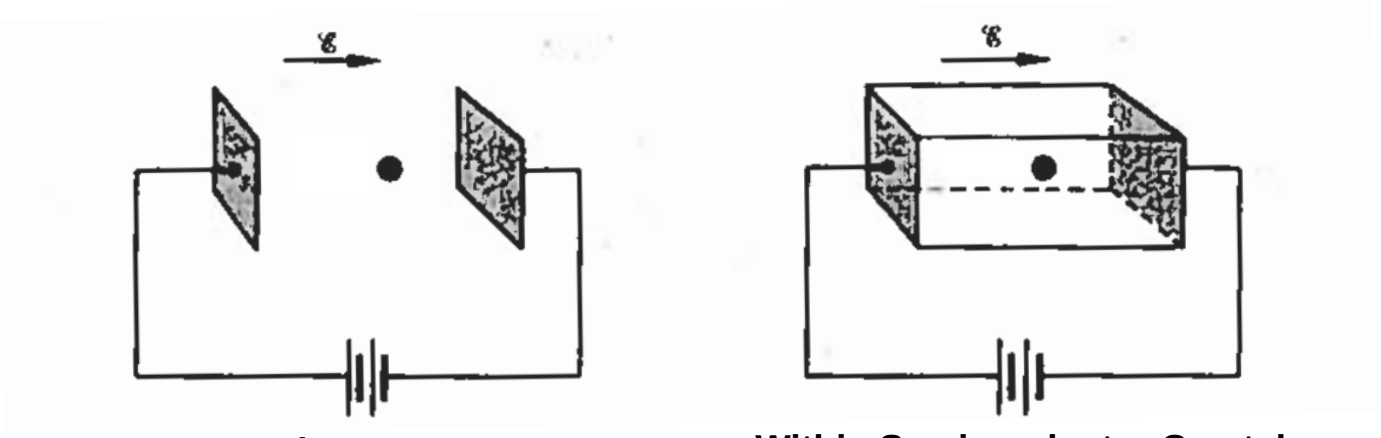
(c) Metal

Charge, Effective Mass

- **Charge**
  - **$|q| = 1.6 \times 10^{-9}$ coulomb**
  - **Electrons: (–), Holes: (+)**

- **Effective mass**
  - **What is the mass of electron?**
  - **What parameters determines the mass?**
  - **Is it a constant like *q*?**

Effective Mass



Under vacuum

Within Semiconductor Crystal

$$F = -q\mathscr{E} = m_0 \frac{dv}{dt}$$

$$F = -q\mathscr{E} = m_n^* \frac{dv}{dt}$$

- **Are the electron movements in both conditions identical?**
- **Disturbances**
- **What is the most accurate way to describe the motion of carriers?**
- **Effective mass**
  - **Internal crystalline fields**
  - **Quantum mechanical effects**
- *"It allows us to conceive of electrons and holes as **quasi-classical particles** and to employ **classical particle relationships** in most device analysis."*

Effective Mass

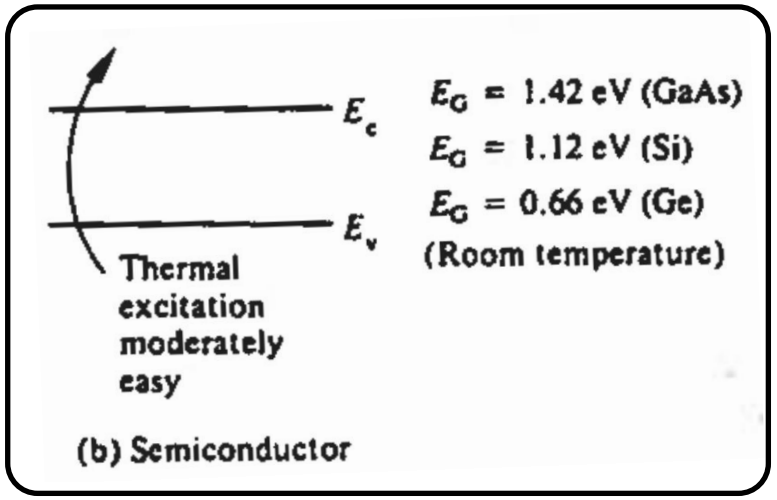
Table 2.1 Density of States Effective Masses at 300 K.

Material	m_n^*/m_0	m_p^*/m_0
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

- **Are m_n^*, m_p^* material dependent?**
  - **Crystallin structure**
  - **Atomic distance(s)**
  - **Temperature**

Carrier Numbers in Intrinsic Material

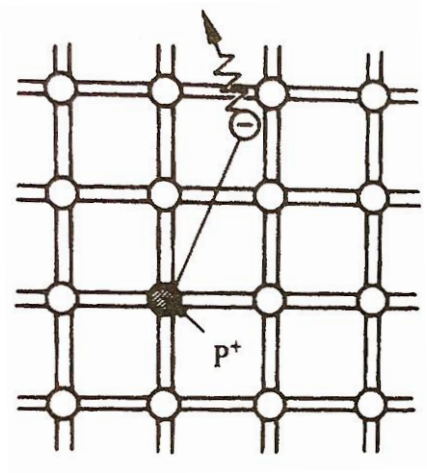
- **Intrinsic semiconductor**
  - Pure semiconductor with *insignificant* amount of impurity atoms
  - Silicon: $n_i = 10^{10}/cm^3$ out of ~$2x10^{23}$ bonds/cm^3 (thermal excitation)
- **Number of carriers**
  - n = # of electrons / cm^3
  - p = # of holes / cm^3
- **In intrinsic semiconductor,**
  - $n = p = n_i$ (under equilibrium)
    - *Why equal?*

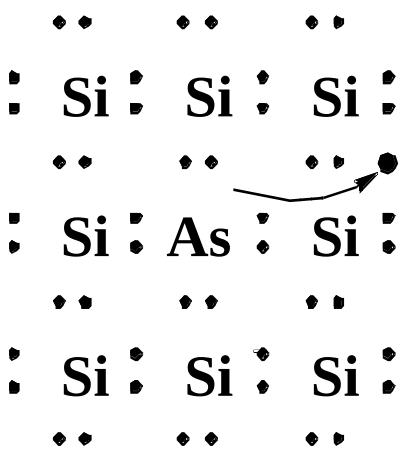


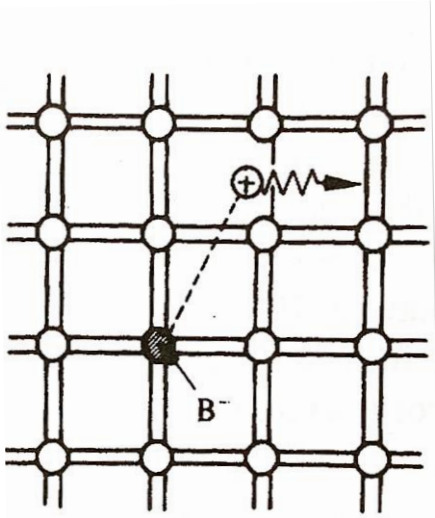
$$\left.\begin{aligned} n_i &\simeq 2 \times 10^6/cm^3 \quad \text{in GaAs} \\ &\simeq 1 \times 10^{10}/cm^3 \quad \text{in Si} \\ &\simeq 2 \times 10^{13}/cm^3 \quad \text{in Ge} \end{aligned}\right\} \text{at room temperature}$$

Manipulation of Carrier Numbers – *Doping*

- **Intrinsic semiconductor does not have enough carriers (i.e. low conductivity)**
- **Intentional addition of impurities**







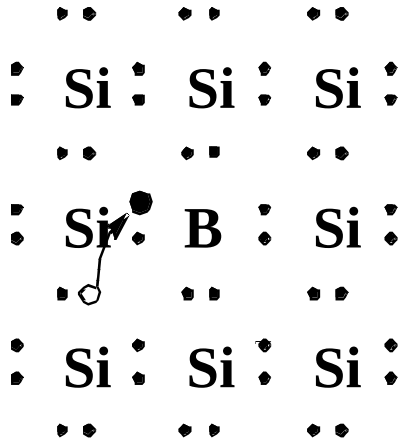


Table 2.2 Common Silicon Dopants. Arrows indicate the most widely employed dopants.

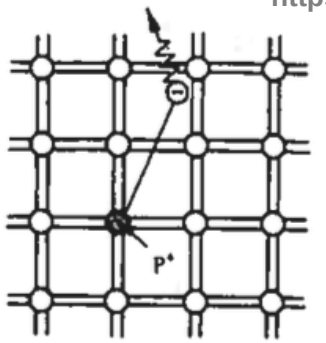
Donors (Electron-increasing dopants)		*Acceptors (Hole-increasing dopants)*	
P ← As ← Sb	Column V elements	B ← Ga In Al	Column III elements

Manipulation of Carrier Numbers – *Doping*

Group →	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period ↓																			
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc		22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
				*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
				**	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

https://en.wikipedia.org/wiki/Periodic_table

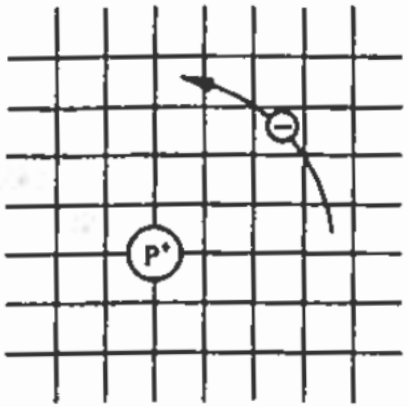
- **# of valence electrons**
- **”weakly bound” electrons**
  - ***How weakly is it bound?***



Manipulation of Carrier Numbers – *Doping*

- **Binding energy**
  - **How much energy would you need to generate carriers from dopants?**

- **Binding energy (E_b) of the fifth doner electron**



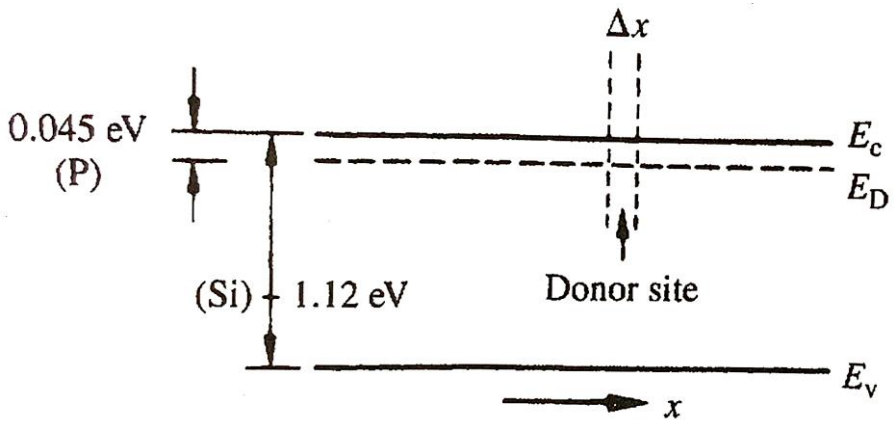
Pseudo-hydrogen atom model for the donor-site bond.

$$E_B \simeq -\frac{m_n^* q^4}{2(4\pi K_S \varepsilon_0 \hbar)^2} = \frac{m_n^*}{m_0}\frac{1}{K_S^2} E_{H|n=1} \simeq -0.1 \text{ eV}$$

Manipulation of Carrier Numbers – *Doping*

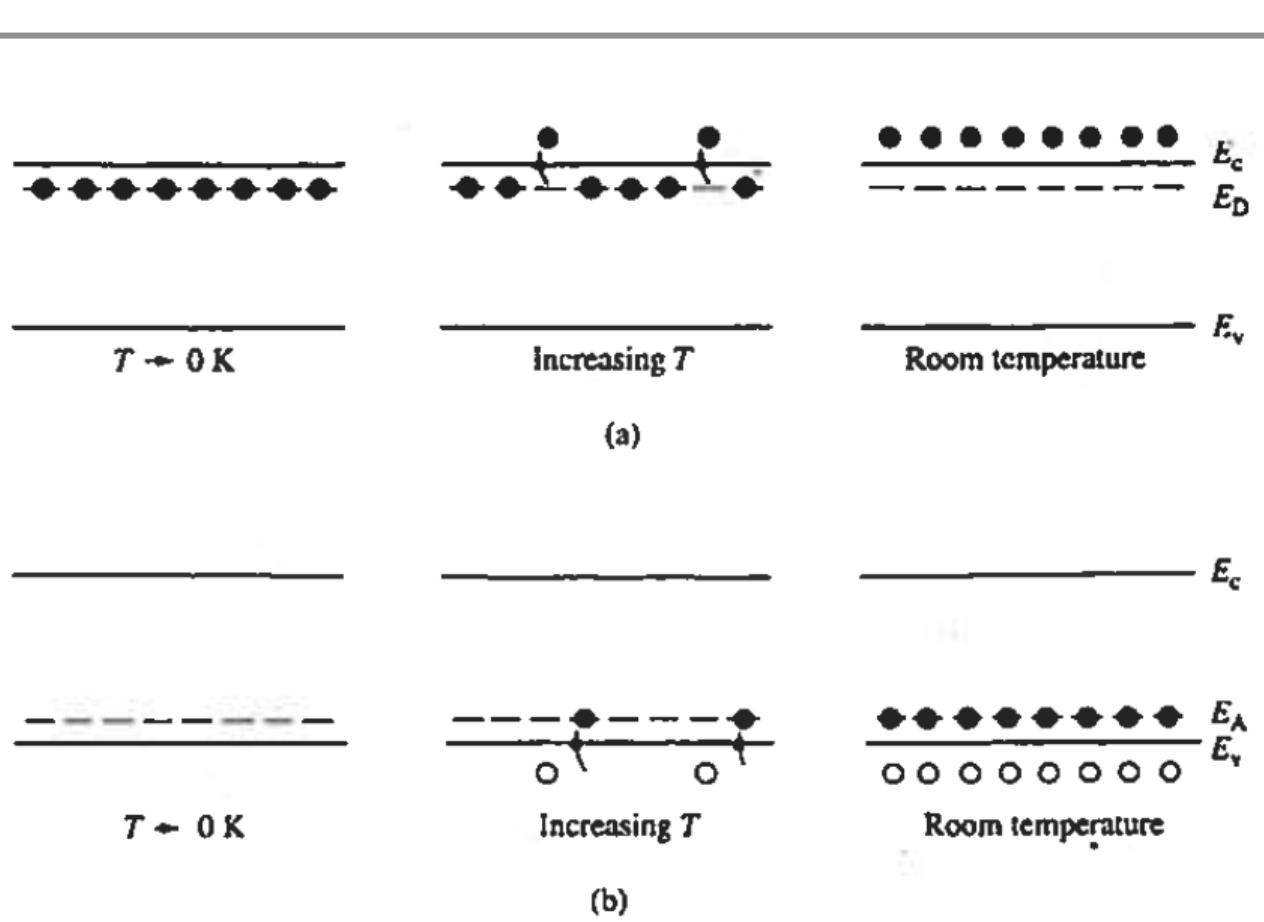
Table 2.3 Dopant-Site Binding Energies.

Donors	$\lvert E_B \rvert$	*Acceptors*	$\lvert E_B \rvert$
Sb	0.039 eV	B	0.045 eV
P	0.045 eV	Al	0.067 eV
As	0.054 eV	Ga	0.072 eV
		In	0.16 eV



- **~5% of Si E_G (bandgap)**
  - **So much easier to generate carriers from dopants than in pure silicon!**
- **Donor energy level (E_D)**
  - $E_D = E_C - |E_B|$
  - **Dashed lines? localization**
- **Acceptor energy level (E_A)**
  - **The same in the opposite direction**

Manipulation of Carrier Numbers – *Doping*



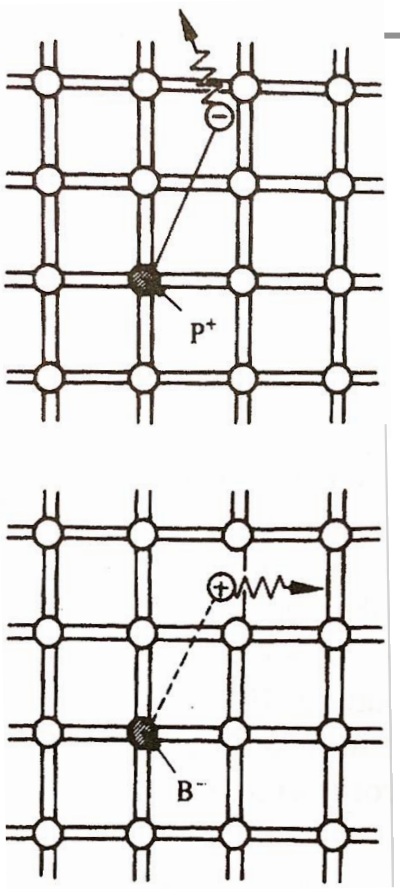


Figure 2.13 Visualization of (a) donor and (b) acceptor action using the energy band model.

- **Small thermal energy (>E_B) would be required for carrier generation.**
- **k_BT = 0.0259 eV (T=300K)**

Average thermal energy of an electron

Carrier-Related Terminology

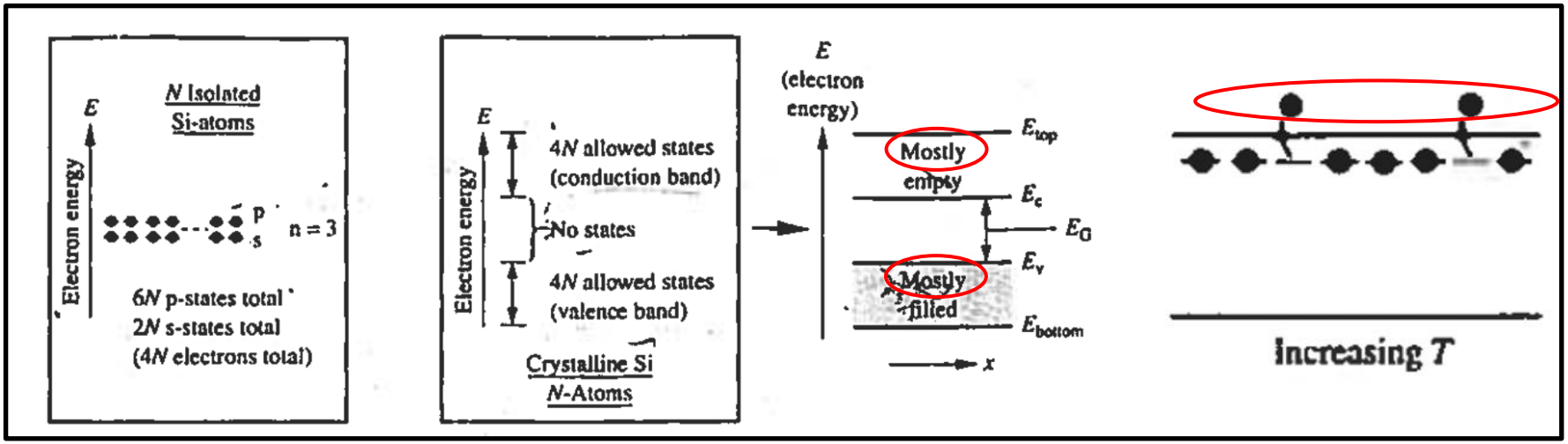
- **Dopants**
- **Intrinsic semiconductor**
- **Extrinsic semiconductor**
- **Donor**
- **Acceptor**
- **n-type material (or semiconductor)**
- **p-type semiconductor**
- **Majority carriers**
- **Minority carriers**

State and Carrier Distributions

- **We've covered the followings so far:**
  - **How the semiconductor is formed from atoms to crystal**
  - **Where intrinsic carriers are located**
  - **How the carriers are generated by introducing dopants**

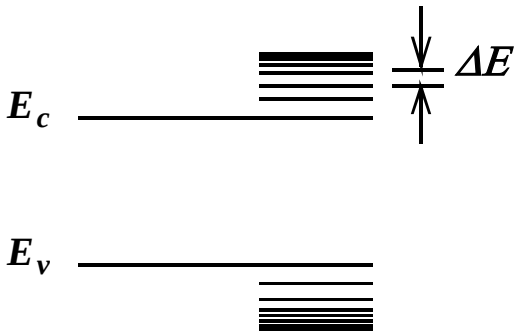
- **Next is, in order to explain how the carriers respond to different electrostatic condition (voltage input), we must understand the followings:**
  - **Precisely how much is the carrier concentration that can contribute to current flow?**
  - **Distribution of carriers as a function of energy**

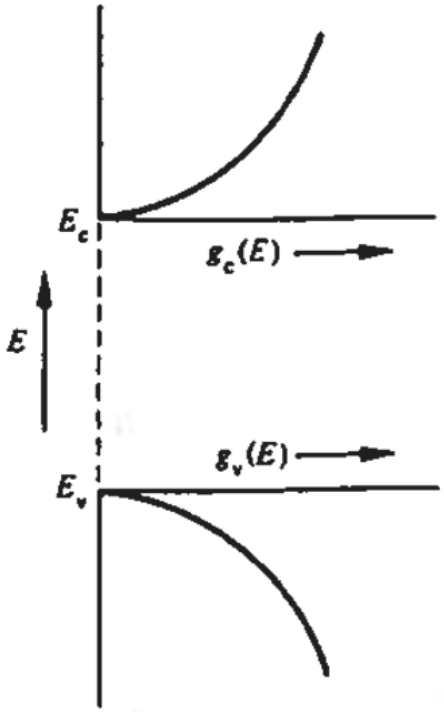
Density of States (DOS)



- Only discussed how many allowed states in atoms in the crystal
- Haven't talked about **the distribution of 'allowed states' in energy**.
- **Density of states (DOS)** – *energy distribution of states*
  - ***Quantum-Mechanical analysis…***

Density of States (DOS)





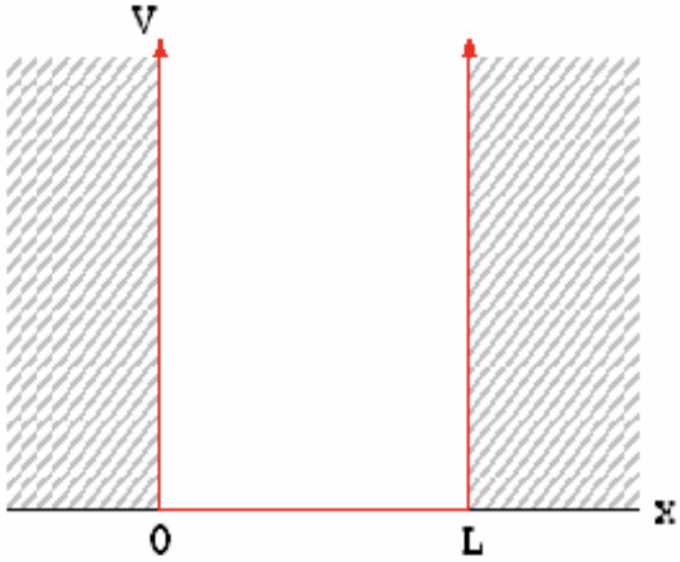
$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}, \qquad E \geq E_c$$

$$g_v(E) = \frac{m_p^* \sqrt{2m_p^*(E_v - E)}}{\pi^2 \hbar^3}, \qquad E \leq E_v$$

# of energy states
per unit volume(cm^3)–unit energy (eV)

- **Increasing # of energy states with square root relationship**
- $g_c(E)dE$: # of conduction band energy states for conduction band electrons per volume (cm^3) within energy level from E and $E+dE$.
- Valence band states
  - Similar for holes in valence band; Effective mass difference

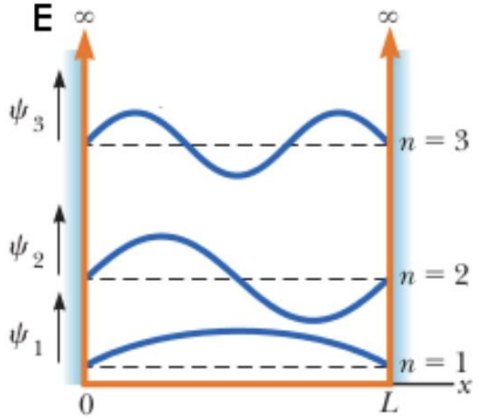
Density of States (DOS)



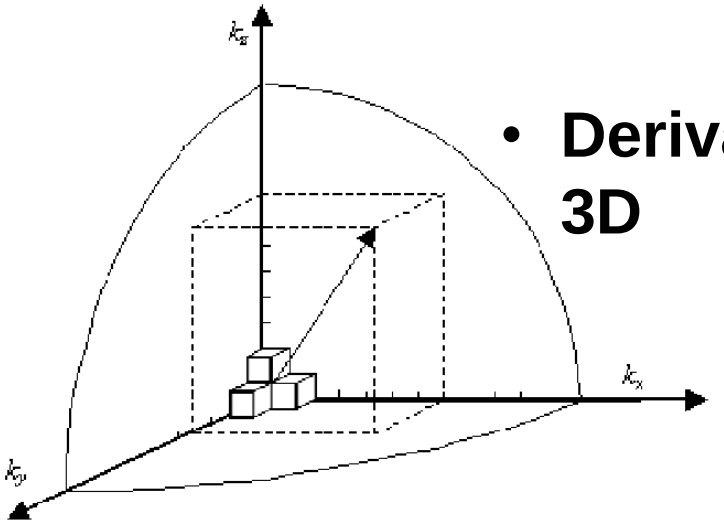
Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+k^2\psi = 0 \quad where \;\; k=\sqrt{\frac{2mE}{\hbar^2}}$$



https://sites.psu.edu/physics/2017/02/10/how-to-sound-smart-101-quantum-mechanics-but-mostly-quantum-tunneling/



- **Derivation over 3D**

Density of States (DOS)

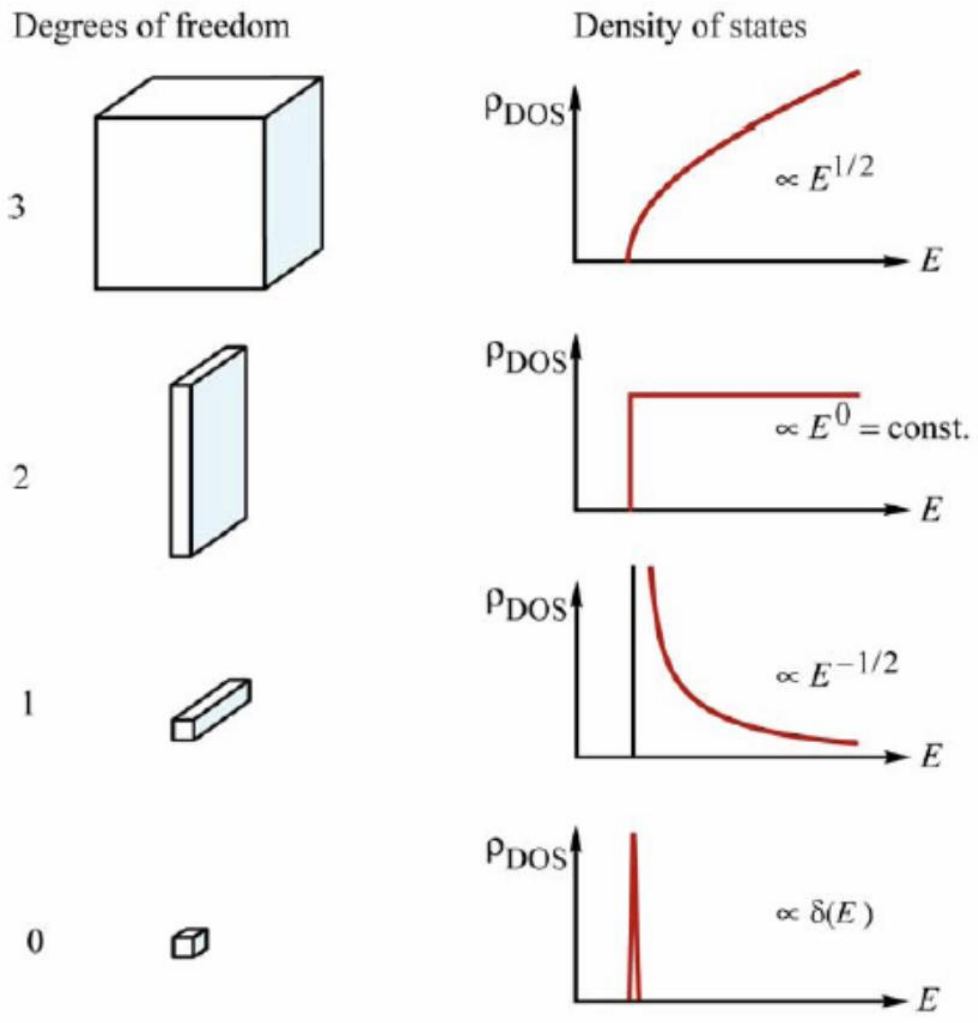


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

The Fermi Function

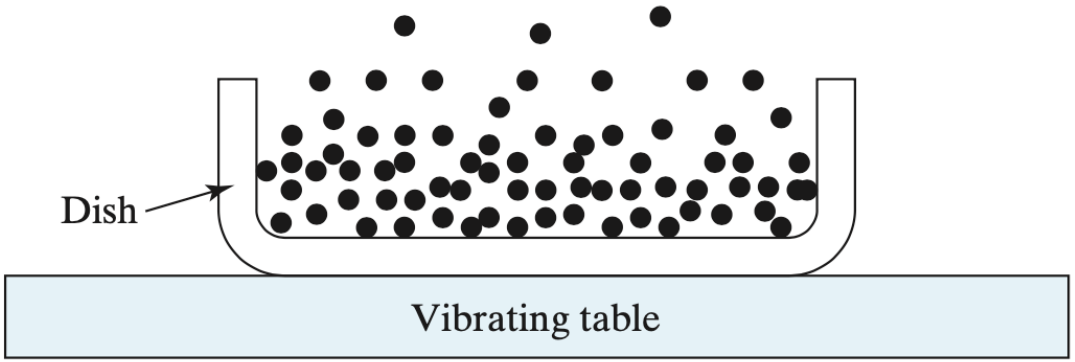


FIGURE 1–17 Elevations of the sand particles in the dish on a vibrating table represent the energies of the electrons in the conduction band under the agitation of thermal energy.

- **With thermal agitation, there is a certain probability for the particles to occupy different heights**
- **The particles = Carriers**
- **Height = Energy levels**

The Fermi Function

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

E_F: Fermi level
k: Boltzmann constant
T: Absolute temperature

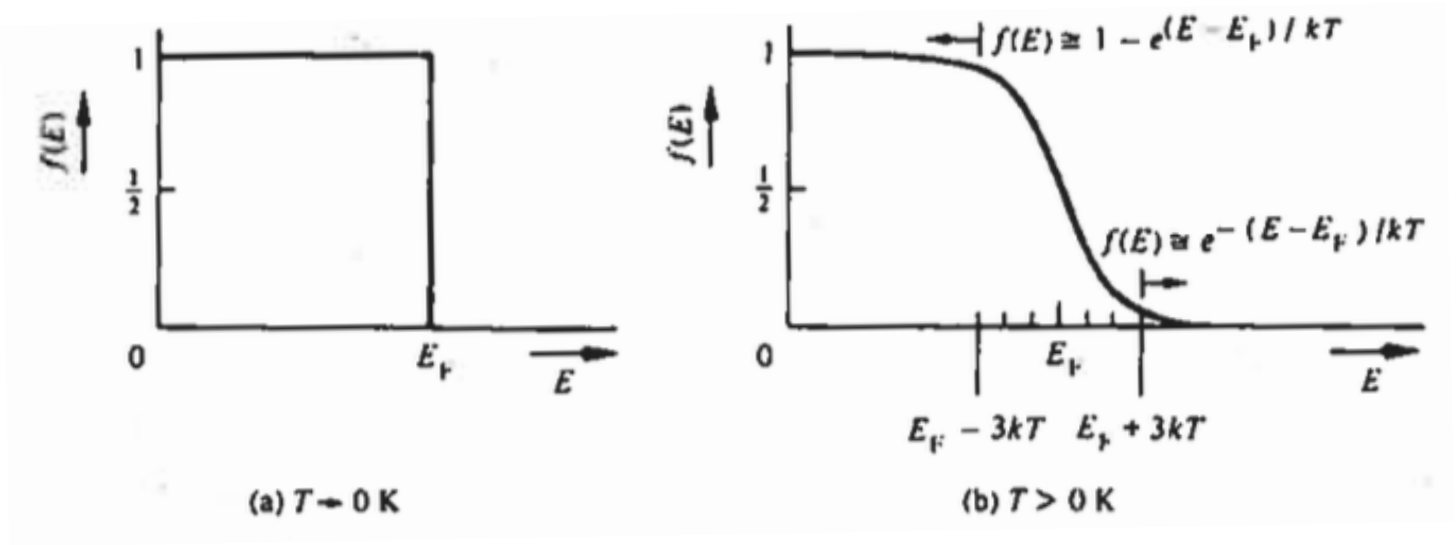
- **Fermi function, *f(E)***
  - **How many of the existing states at energy level *E* can be filled (occupied) with an electron**
  - **Probability distribution function**

The Fermi Function

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

E_F: Fermi level
k: Boltzmann constant
T: Absolute temperature

- *If T=0 K?*
- $f(E_F) = f(E=E_F) =$ *?*
- *If* $E \geq E_F + 3kT$? $e^3 \approx 20$. $f(E) \approx \frac{1}{21}$
- **At RT, $3kT$ = 77.7 meV (=0.0777 eV) for Si (cf. Si bandgap = 1.12eV)**



The Fermi Function

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

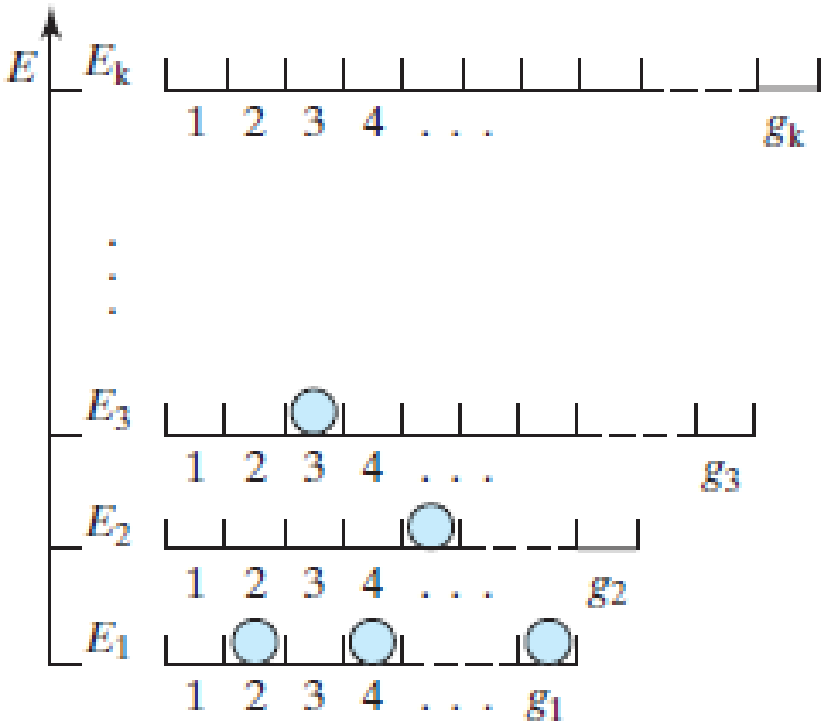
Exercise 2.2

P: The probability that a state is filled at the conduction band edge (E_c) is precisely equal to the probability that a state is *empty* at the valence band edge (E_v). Where is the Fermi level located?

Equilibrium Distribution of Carriers

- Knowing **(1) <u>the distribution of available energy states (DOS)</u>** in conduction band and valence band, and **(2) <u>probability to find the electrons (Fermi function)</u>** at a given energy level, we can now calculate the distribution of electrons.

- DOS x Fermi function
  - $g_c(E) \times f(E)$
  - $g_v(E) \times (1 - f(E))$



From "Modern Semiconductor Devices for Integrated Circuits (C. Hu)"

Equilibrium Distribution of Carriers

- Knowing **(1) <u>the distribution of available energy states (DOS)</u>** in conduction band and valence band, and **(2) <u>probability to find the electrons (Fermi function)</u>** at a given energy level, we can now calculate the distribution of electrons.
- DOS x Fermi function
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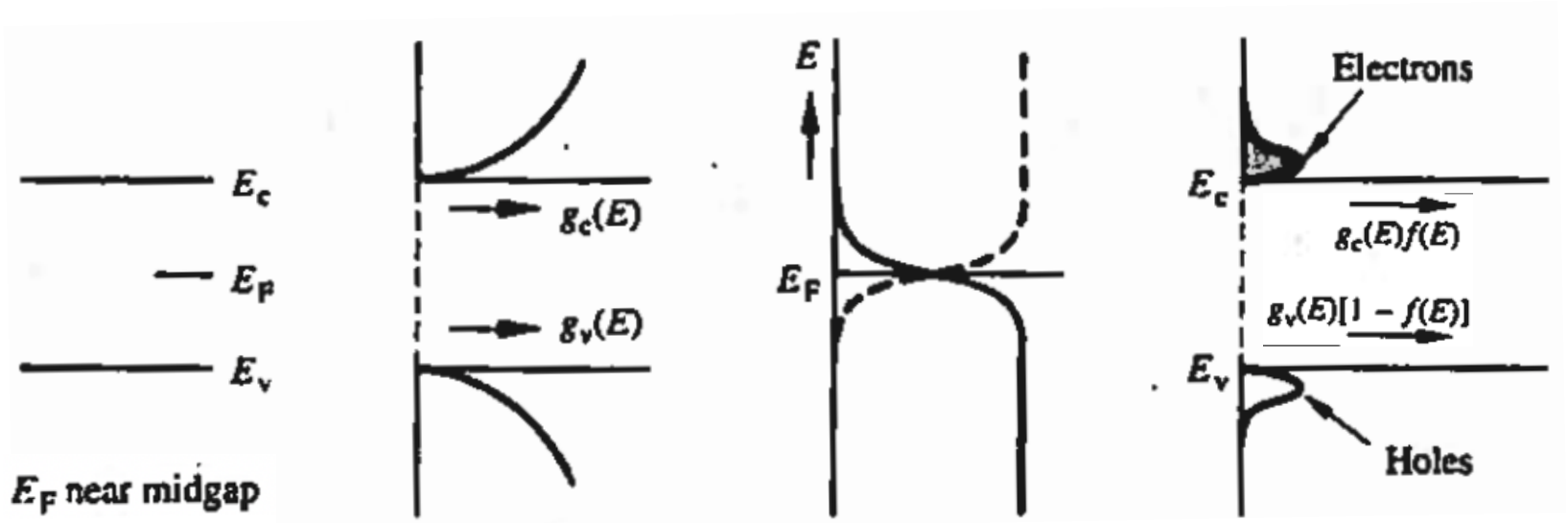
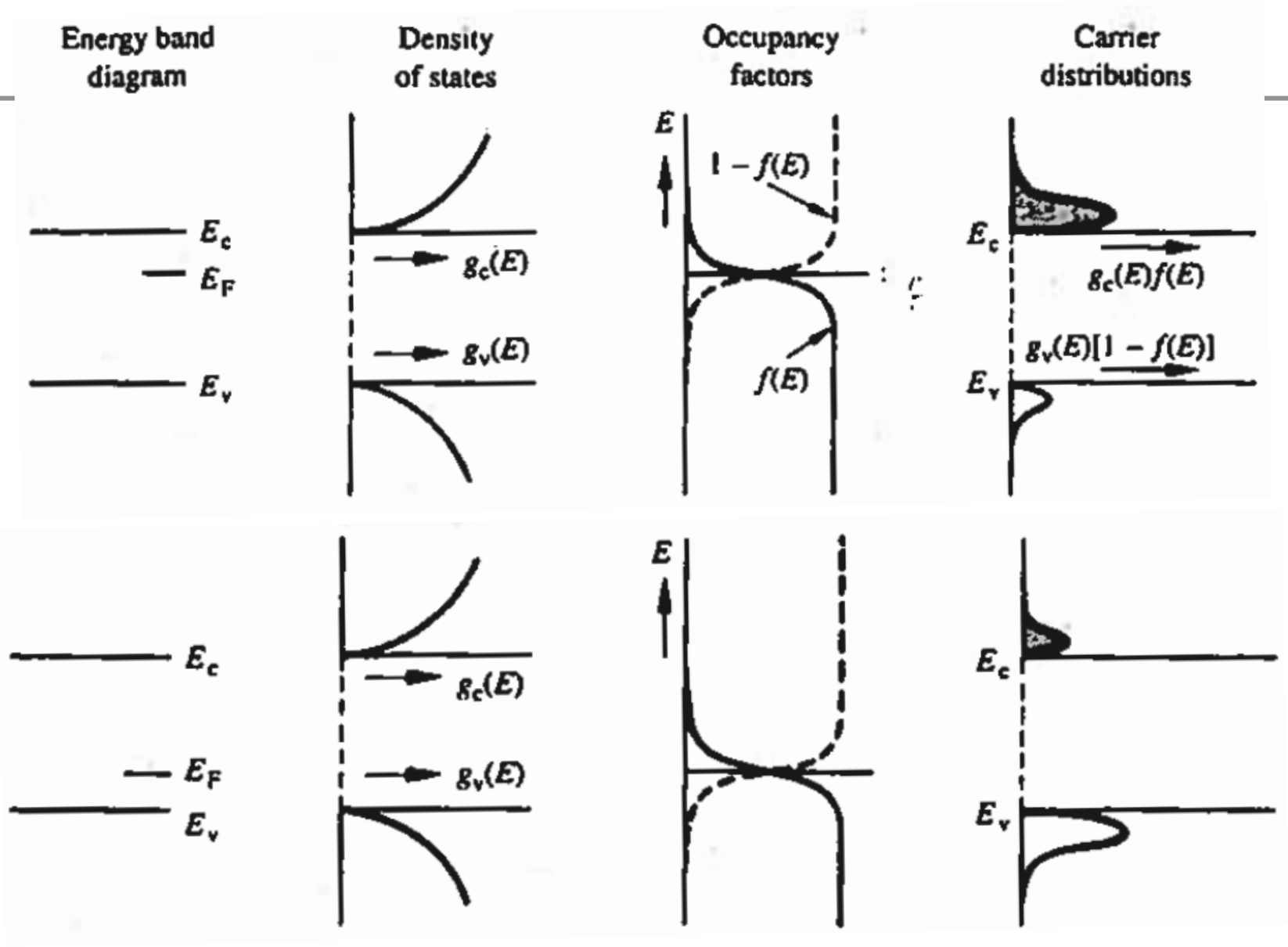
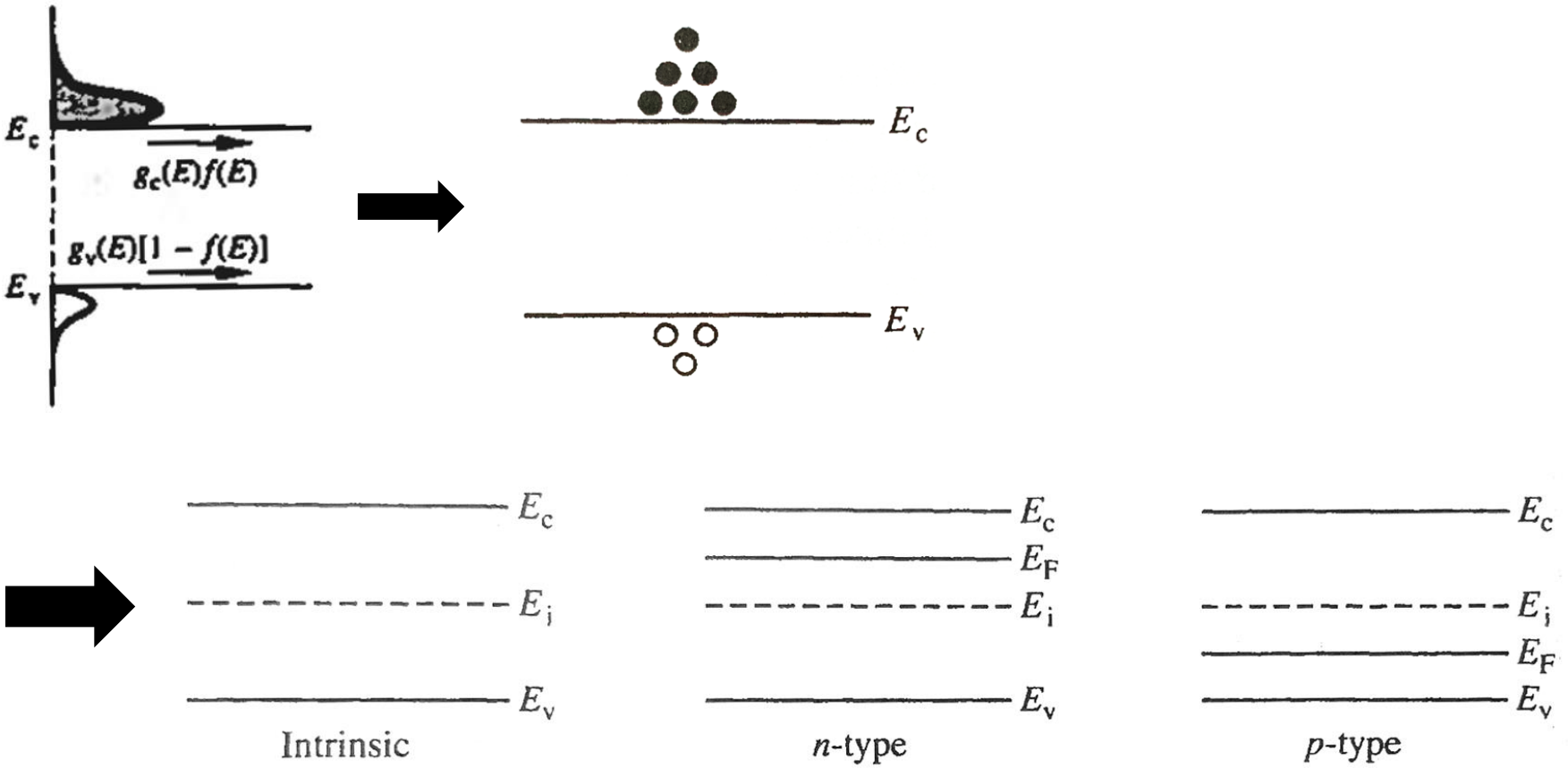


DOS **Fermi function** **Carrier distribution**



- ***What if the Fermi level is NOT at the mid gap?***

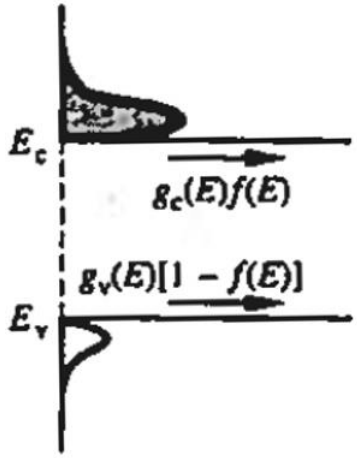
Equilibrium Distribution of Carriers



- **Simplified representation of the distribution of carriers**
  - **Spatial information**

Furmulas for *n* and *p*

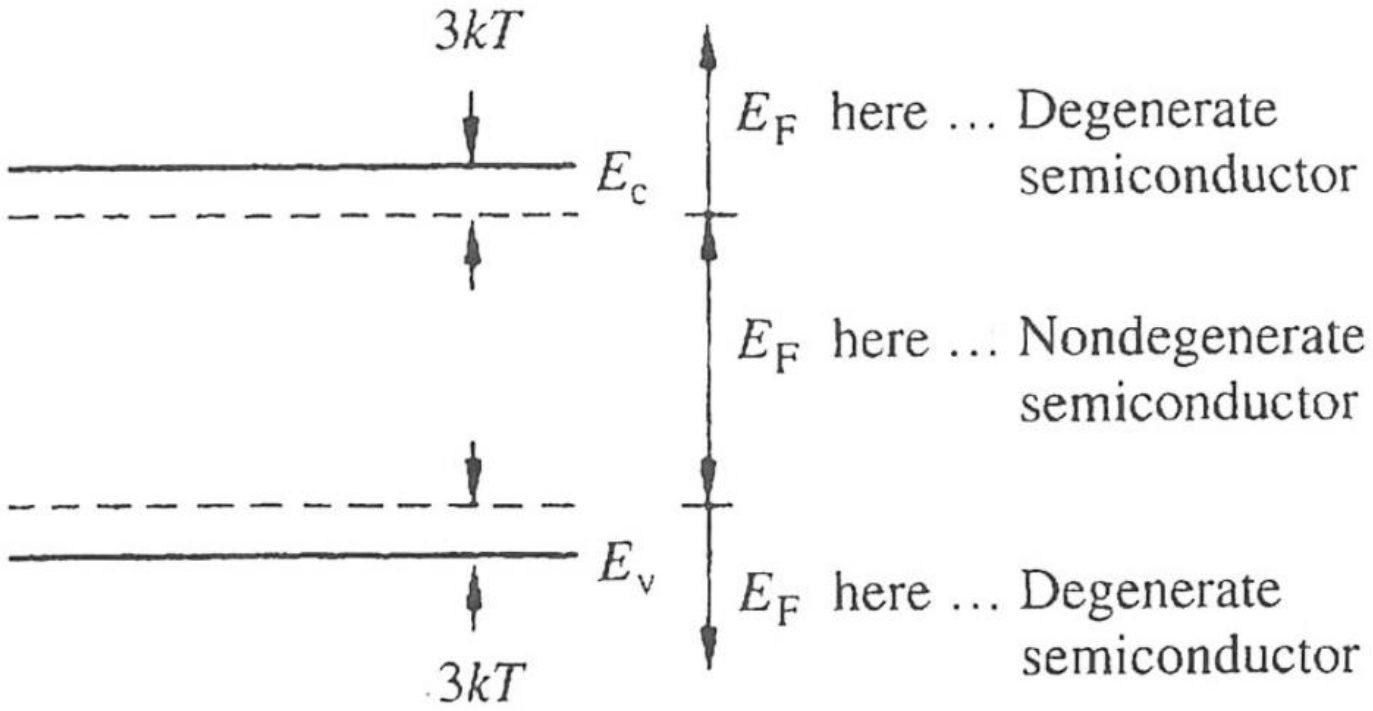
- **Carrier concentration (*n*, *p*)**
  - $g_c(E) \times f(E) \times dE$: # of conduction band electrons per volume (cm^3) within energy level from E and $E+dE$
  - Integration over the entire conduction band
  - $n = \int_{E_c}^{E_{top}} g_c(E) f(E) dE$
  - $p = \int_{E_{bottom}}^{E_v} g_v(E)[1 - f(E)] dE$



$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}, \qquad E \geq E_c$$

$$f(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}} \approx \frac{1}{21} \qquad if\ E_C - E_F \geq 3kT\ (= 0.0259\ eV)$$

Furmulas for *n* and *p*



- **Degenerate semiconductor**
- **Nondegenerate semiconductor**

Furmulas for *n* and *p*

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

$$f(E) \approx e^{-\frac{E-E_F}{kT}} \quad (E_C - E_F \geq 3kT)$$

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

- $n = \int_{E_c}^{E_{top}} g_c(E) f(E) dE$

- $n = N_C e^{-\frac{E_C - E_F}{kT}}$, where $N_C = 2\left[\frac{m_n^* kT}{2\pi\hbar^2}\right]^{\frac{3}{2}}$

Effective density states

- $p = N_V e^{-\frac{E_F - E_v}{kT}}$, where $N_V = 2\left[\frac{m_p^* kT}{2\pi\hbar^2}\right]^{\frac{3}{2}}$