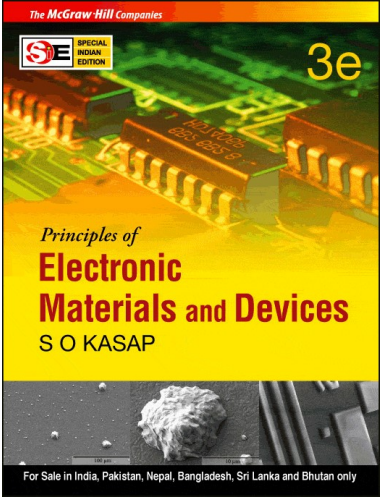


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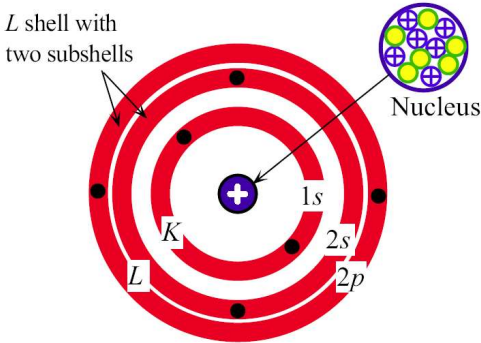
Chapter 4

Modern Theory of Solids

1

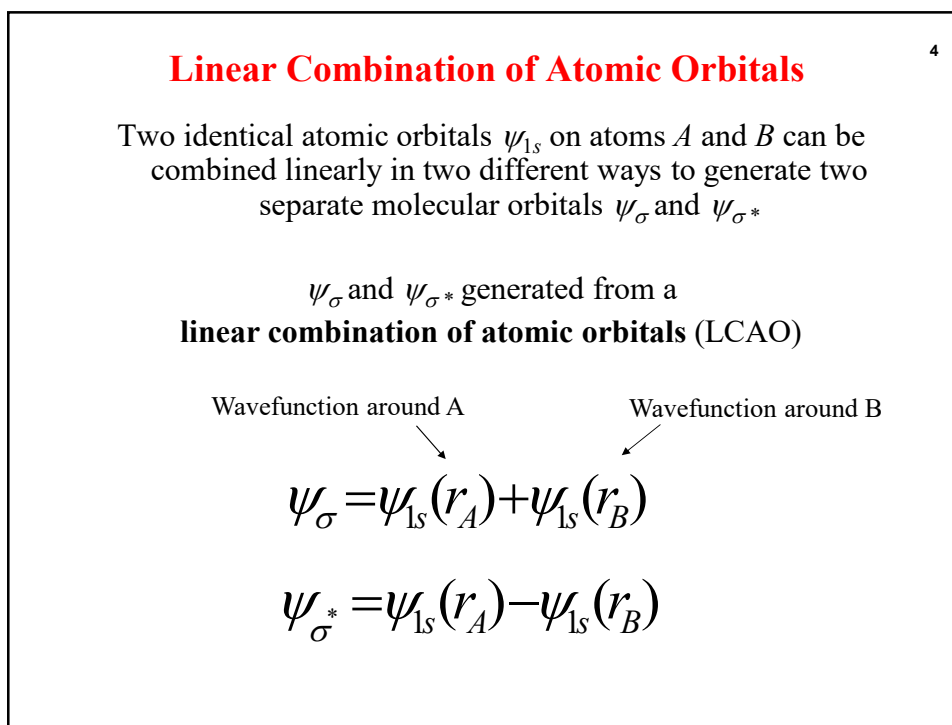
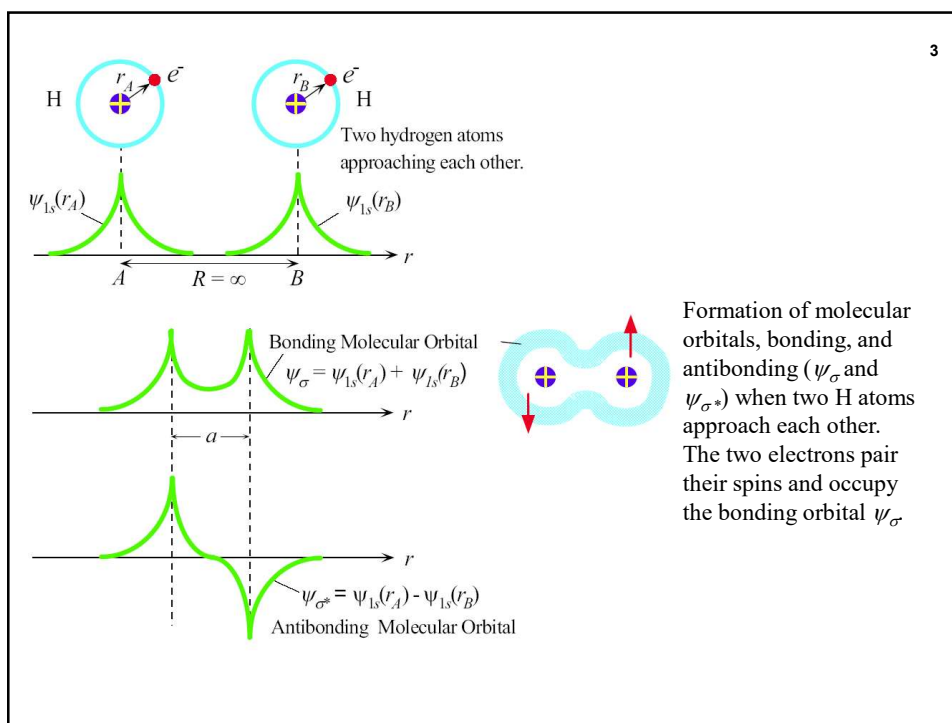
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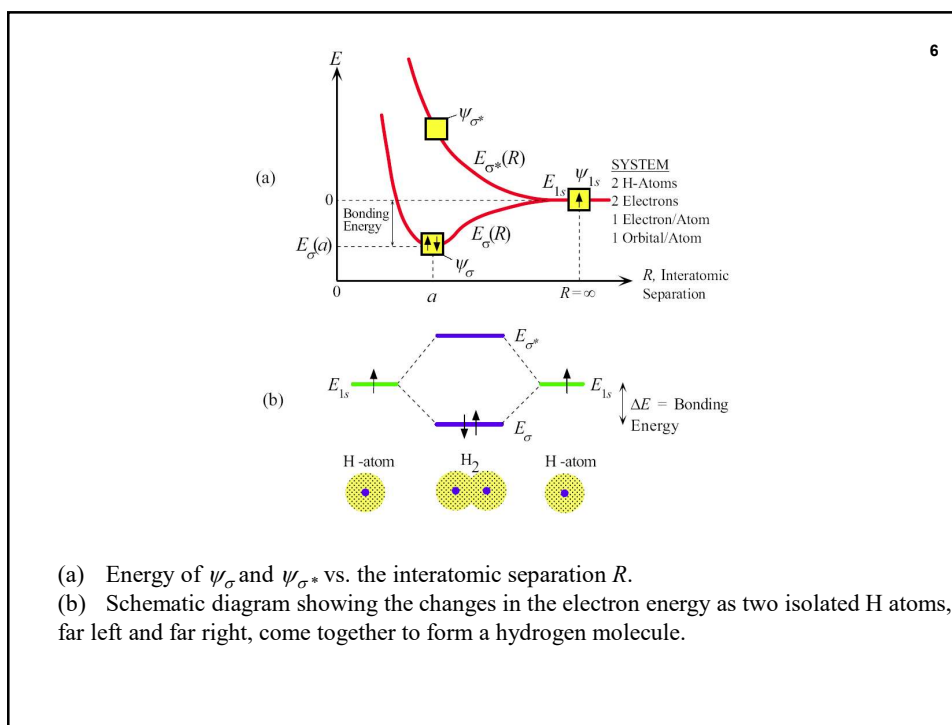
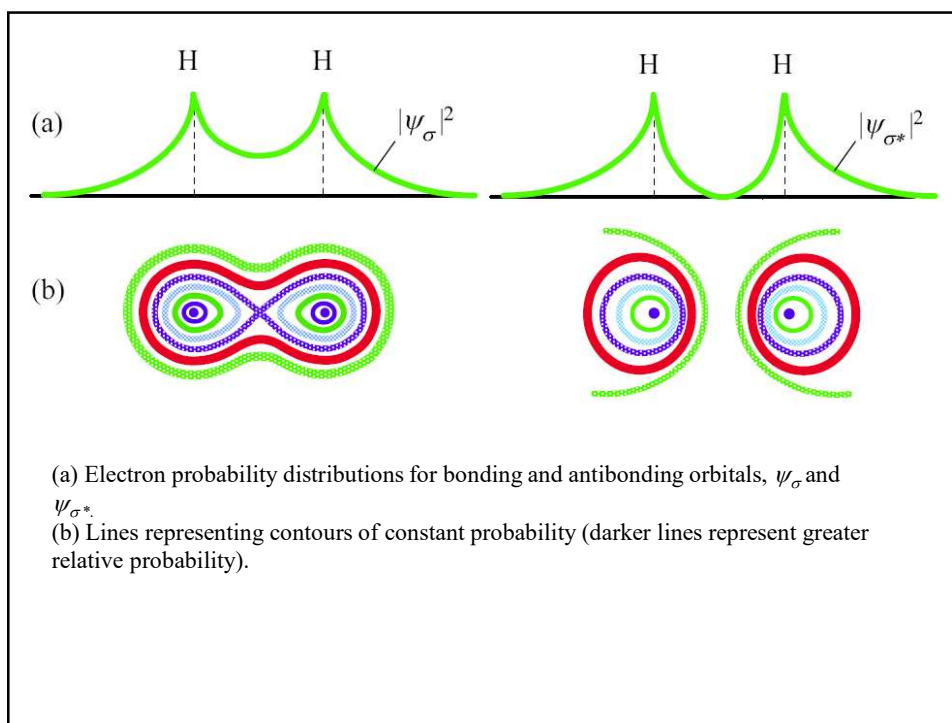
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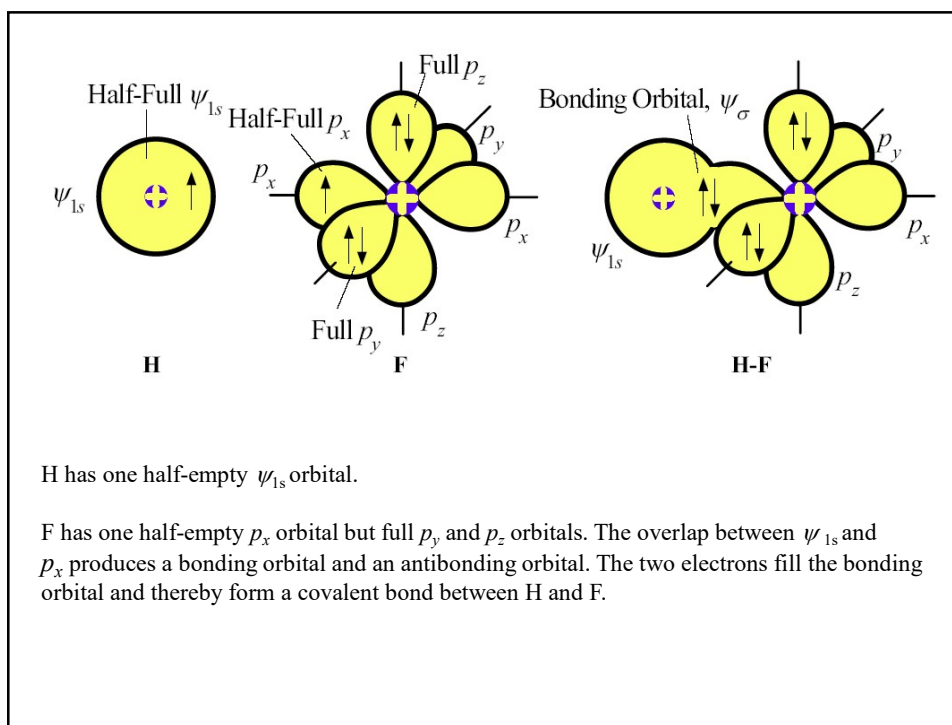
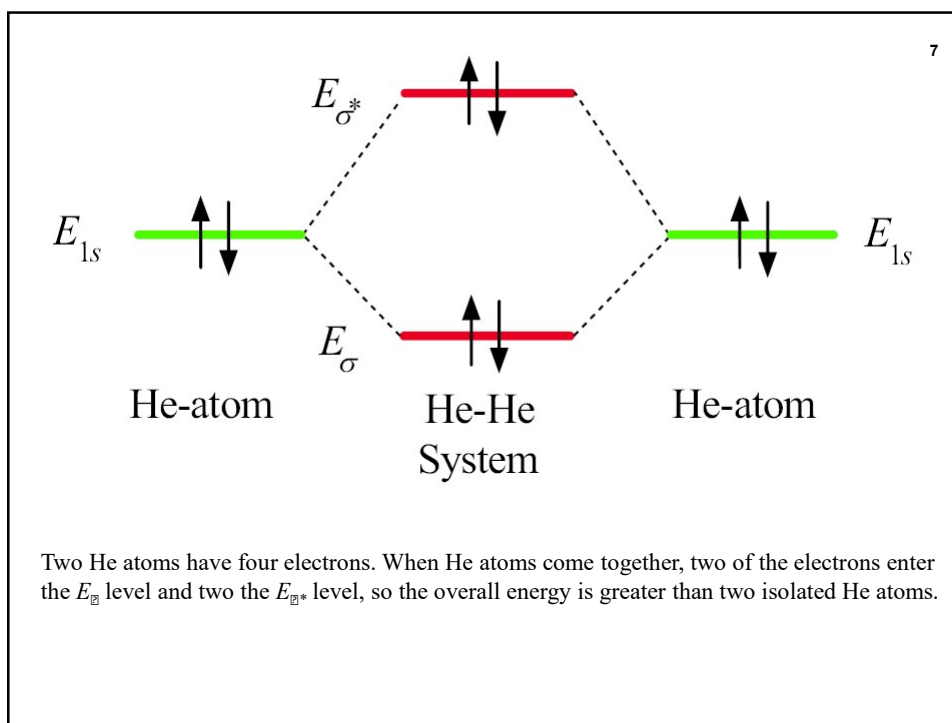


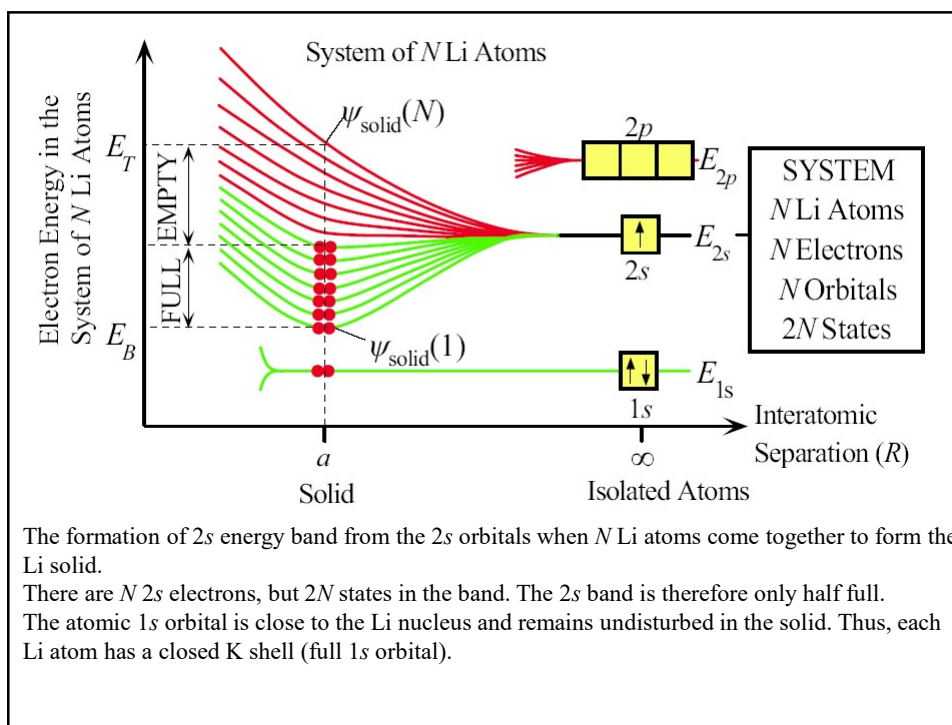
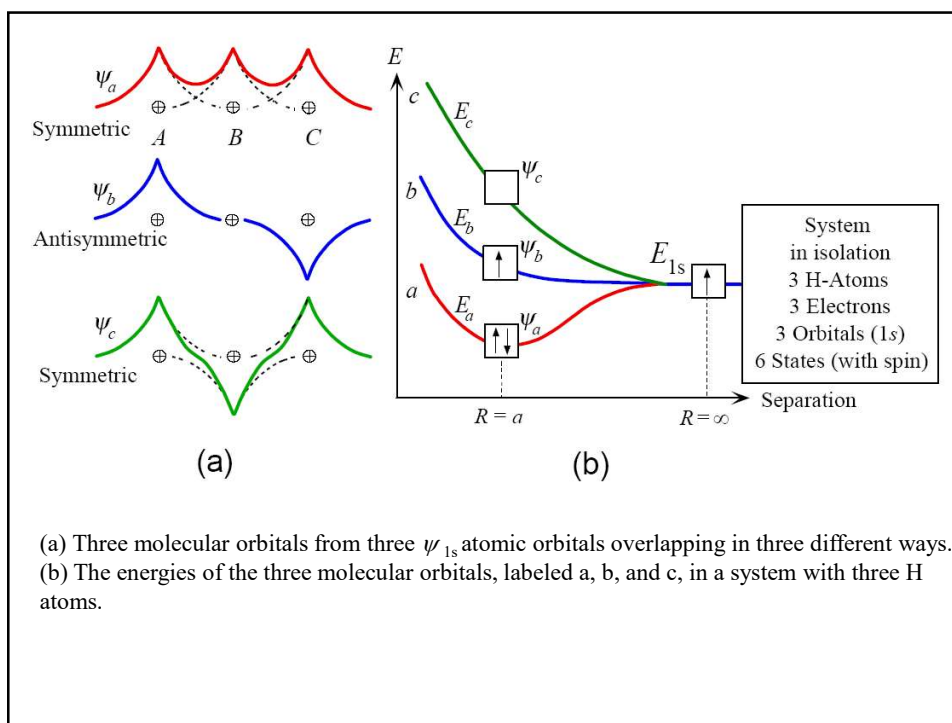
$1s^2 2s^2 2p^2$ or $[\text{He}] 2s^2 2p^2$

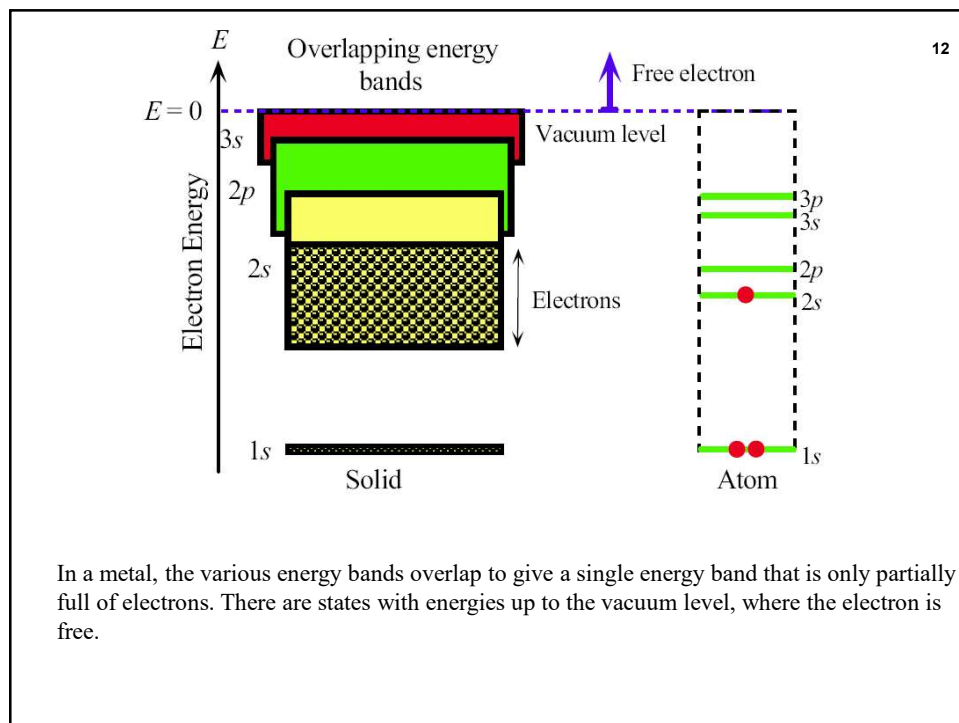
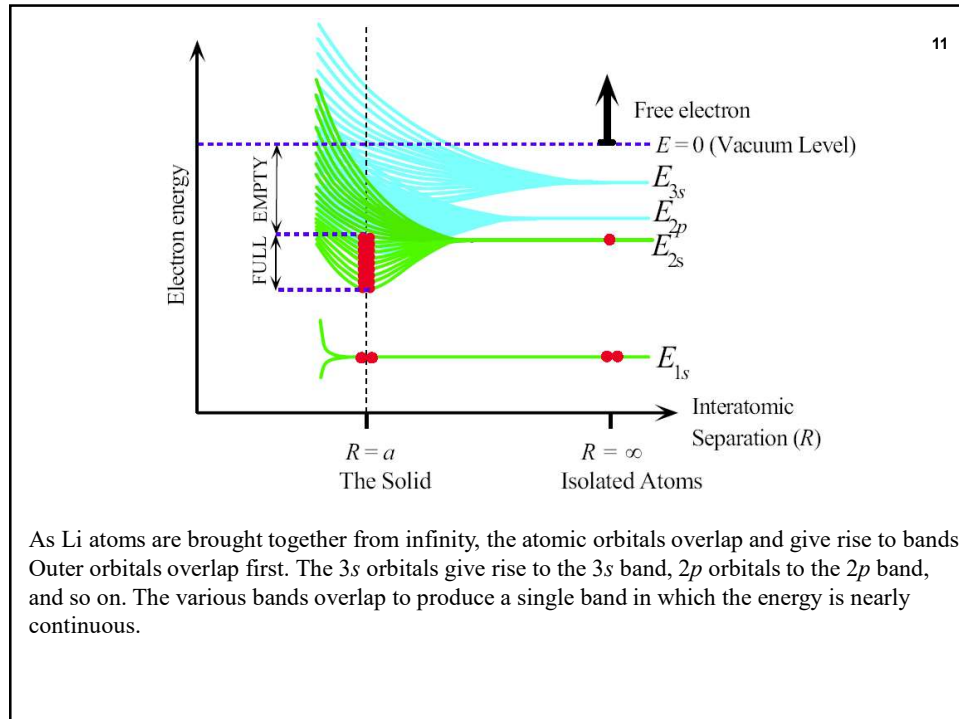
The shell model of the atom in which electrons are confined to live within certain shells and in subshells within shells





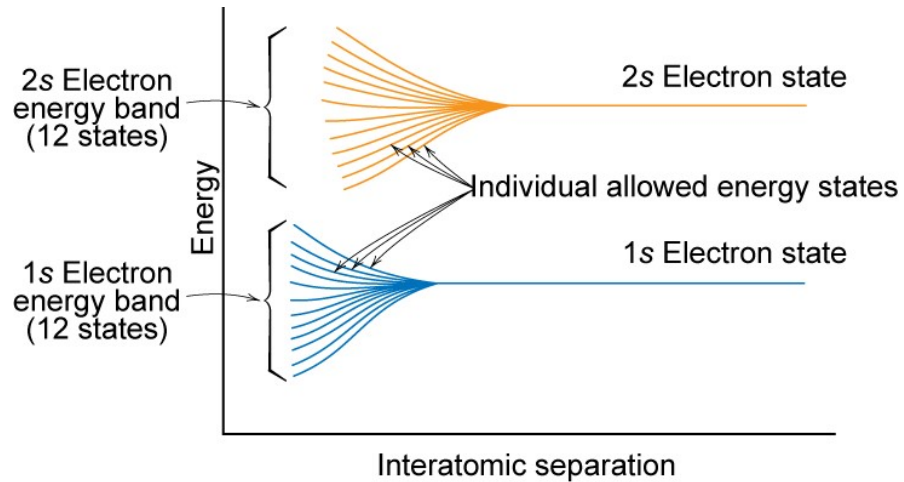






Electron Energy Band Structures

13

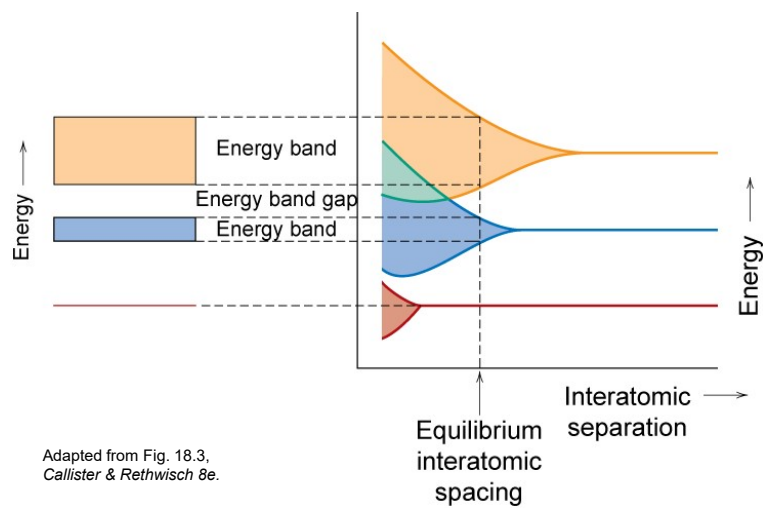


Adapted from Fig. 18.2, Callister & Rethwisch 8e.

13

Band Structure Representation

14



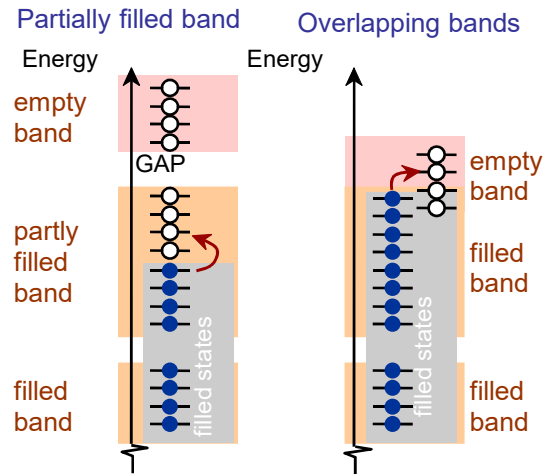
Adapted from Fig. 18.3, Callister & Rethwisch 8e.

14

Conduction & Electron Transport

15

- Metals (**Conductors**):
 - for metals empty energy states are adjacent to filled states.
 - thermal energy excites electrons into empty higher energy states.
 - two types of band structures for metals
 - partially filled band
 - empty band that overlaps filled band

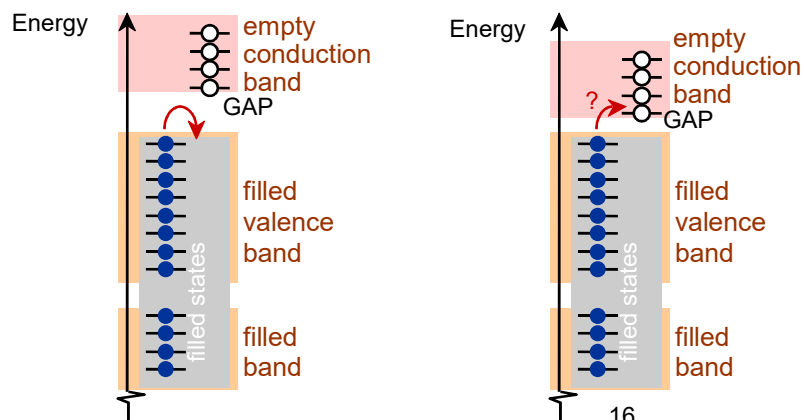


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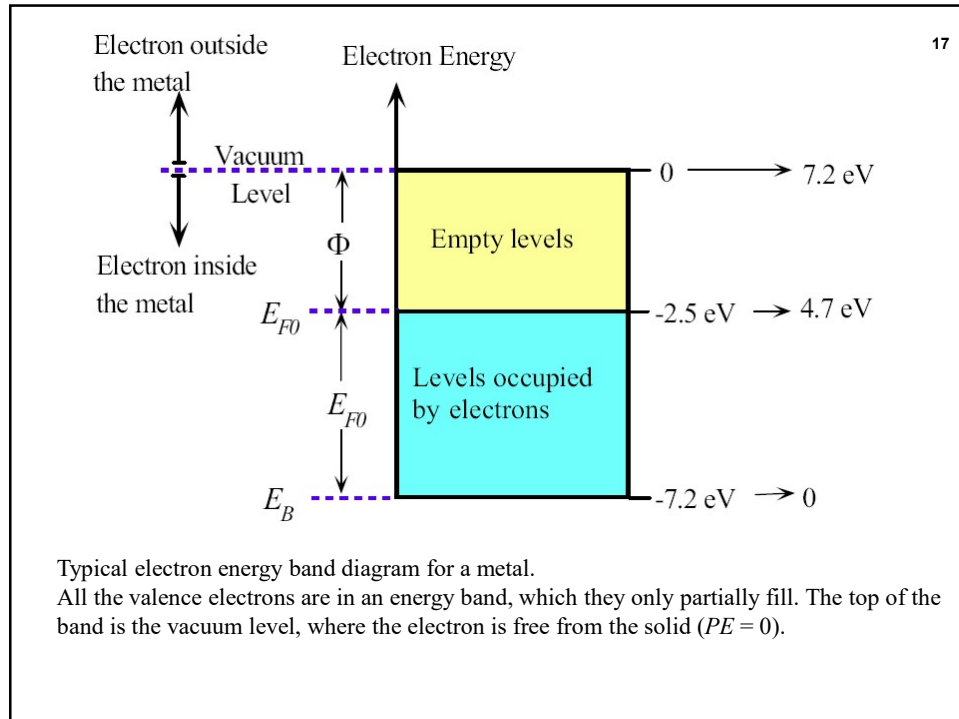
Energy Band Structures: Insulators & Semiconductors

16

- Insulators:
 - wide band gap (> 2 eV)
 - few electrons excited across band gap
- Semiconductors:
 - narrow band gap (< 2 eV)
 - more electrons excited across band gap



16



Work function Φ

18

The energy required to excite an electron from the Fermi level to the vacuum level, that is, to liberate the electron from the metal, is called the **work function Φ** of the metal.

Electron gas in a metal

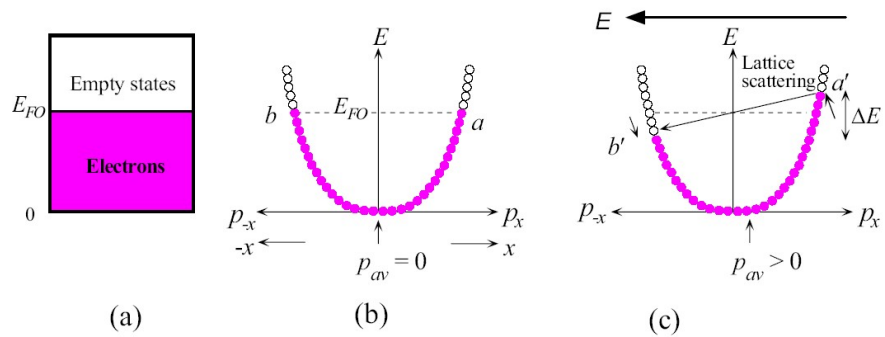
The electrons in the energy band of a metal are loosely bound valence electrons, which become free in the crystal and thereby form a kind of **electron gas** within the crystal. It is this electron gas that holds the metal ions together in the crystal structure and constitutes the metallic bond.

19

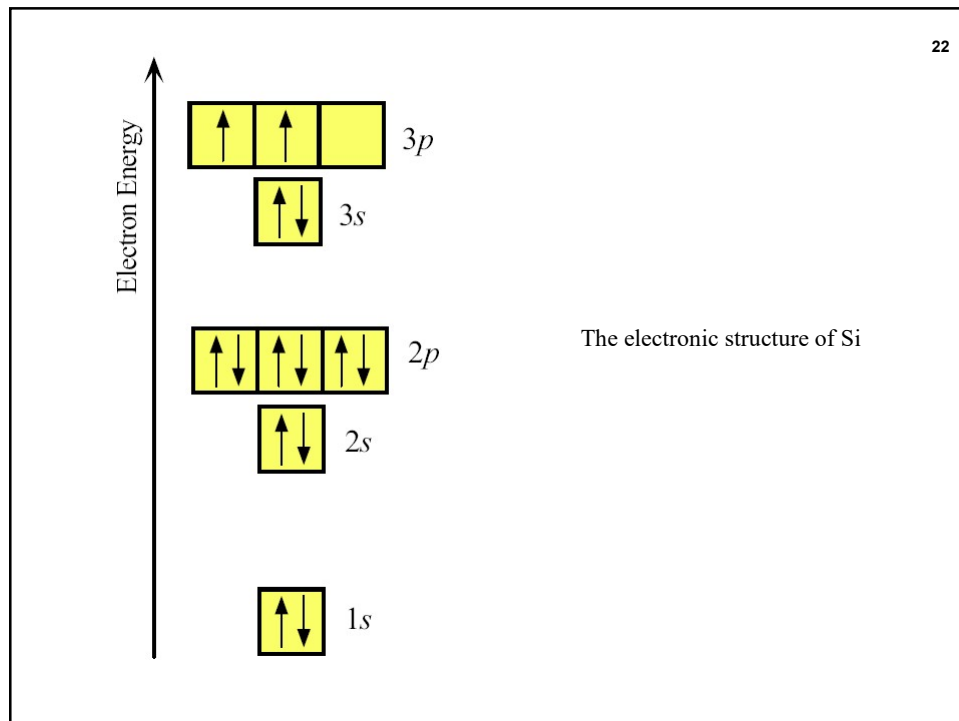
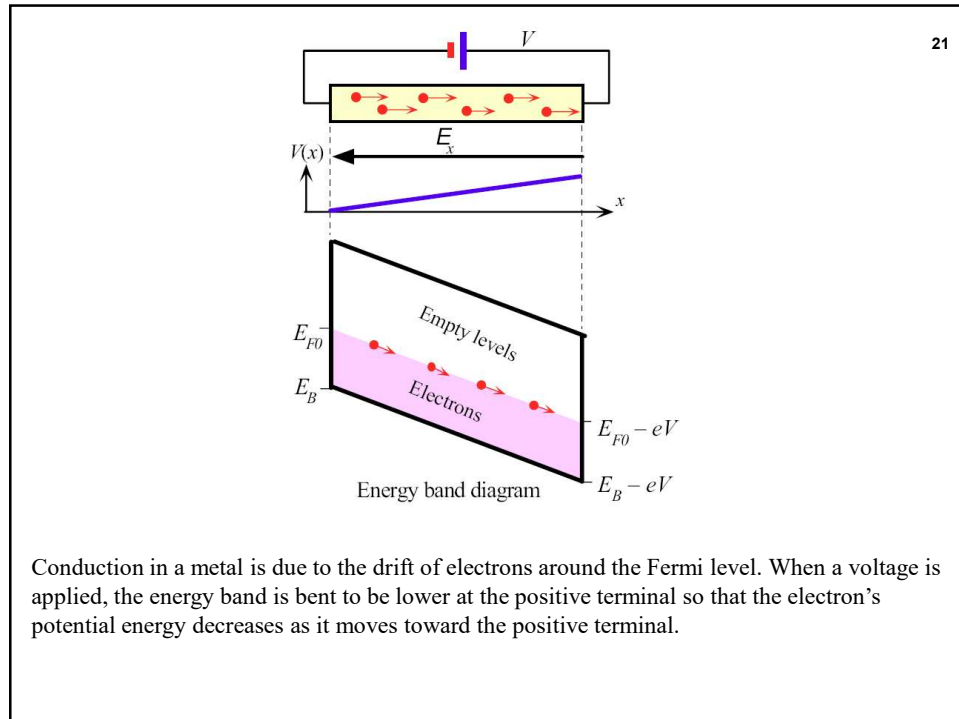
Table 4.1 Fermi energy and work function of selected metals

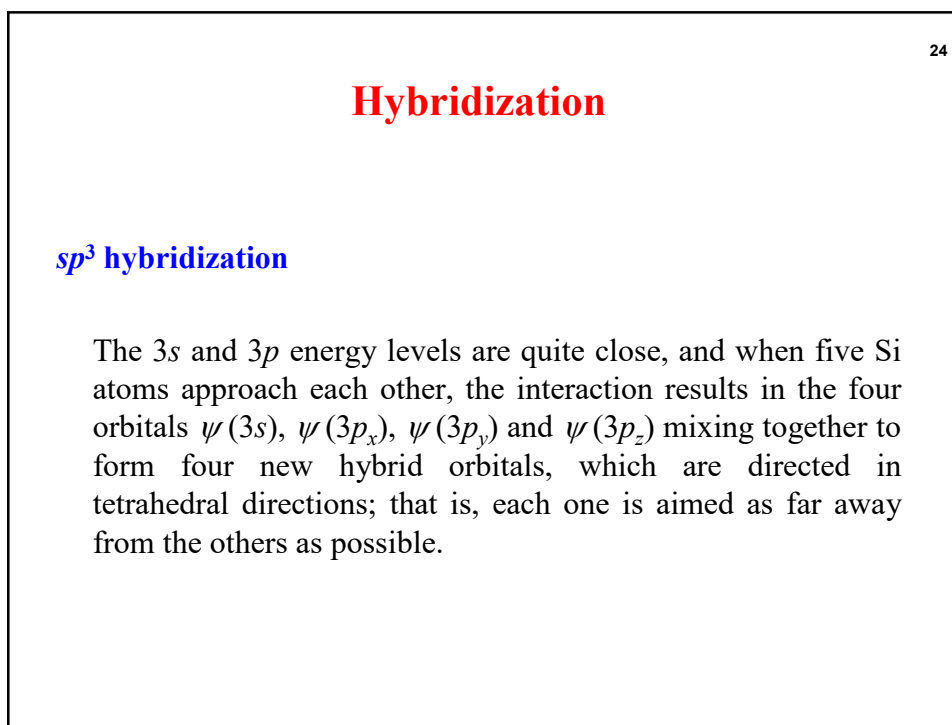
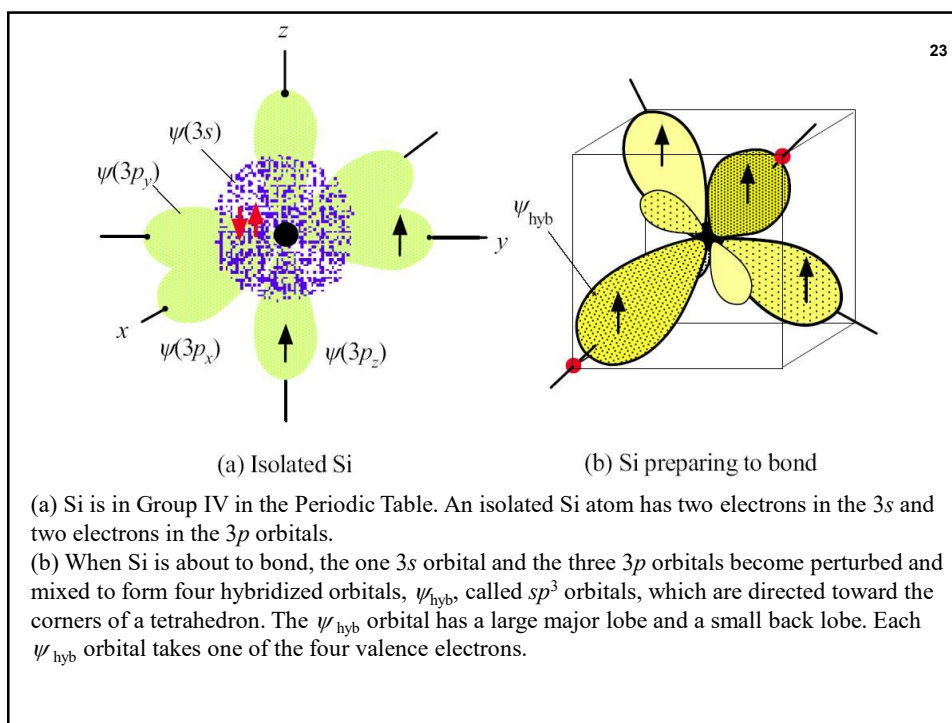
	Metal							
	Ag	Al	Au	Cs	Cu	Li	Mg	Na
Φ (eV)	4.5	4.28	5.0	2.14	4.65	2.3	3.7	2.75
E_{FO} (eV)	5.5	11.7	5.5	1.58	7.0	4.7	7.1	3.2

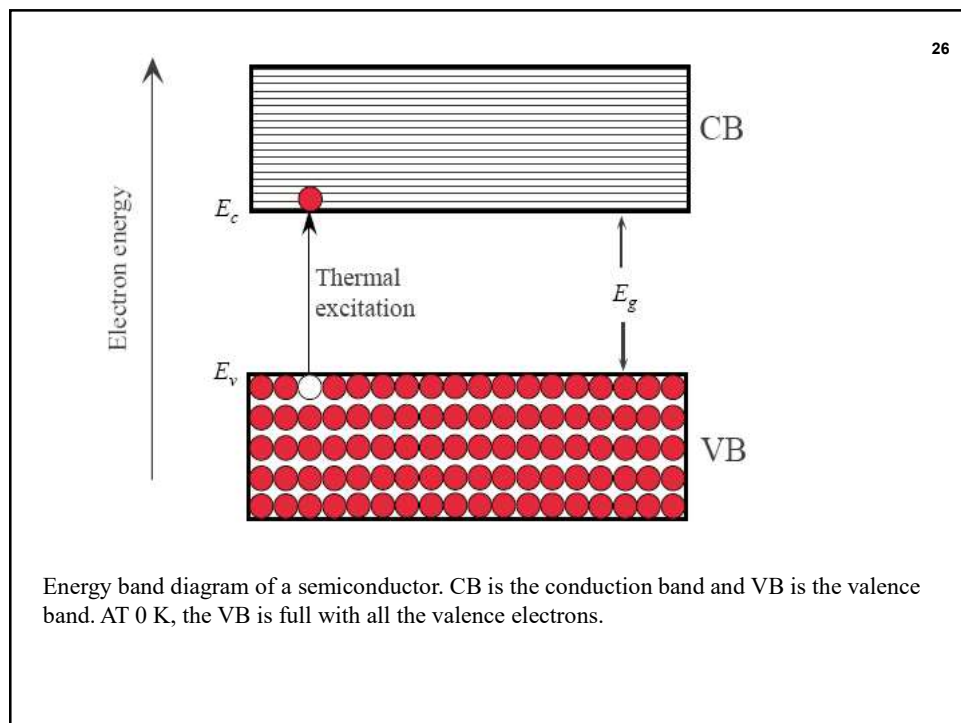
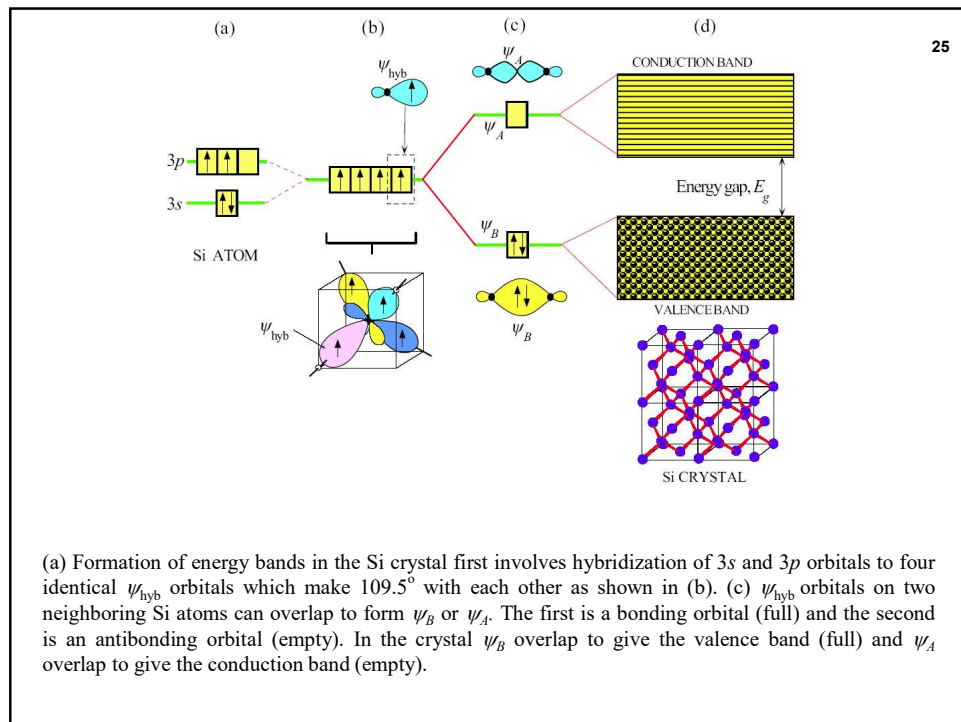
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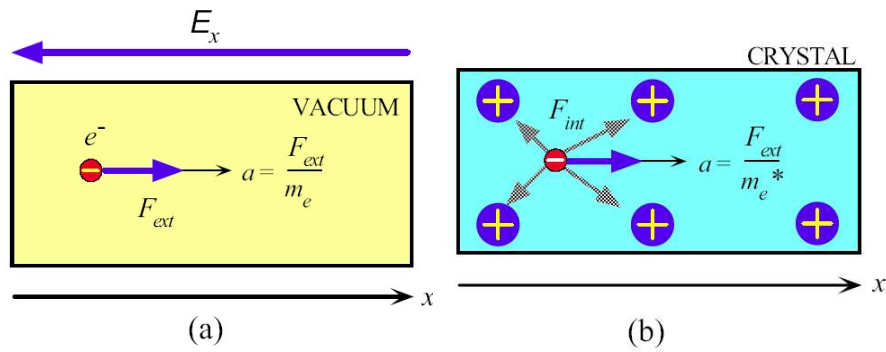
(a) Energy band diagram of a metal. (b) In the absence of a field, there are as many electrons moving right as there are moving left. The motions of two electrons at each energy cancel each other as for a and b . (c) In the presence of a field in the x direction, the electron a accelerates and gains energy to a' where it is scattered to an empty state near E_{FO} but moving in the $-x$ direction. The average of all momenta values is along the $+x$ direction and results in a net electrical current.







27



(a) An external force F_{ext} applied to an Electron in a vacuum results in an acceleration $a_{vac} = F_{ext} / m_e$.

(b) An external force F_{ext} applied to an electron in a crystal results in an acceleration $a_{cryst} = F_{cryst} / m_e^*$

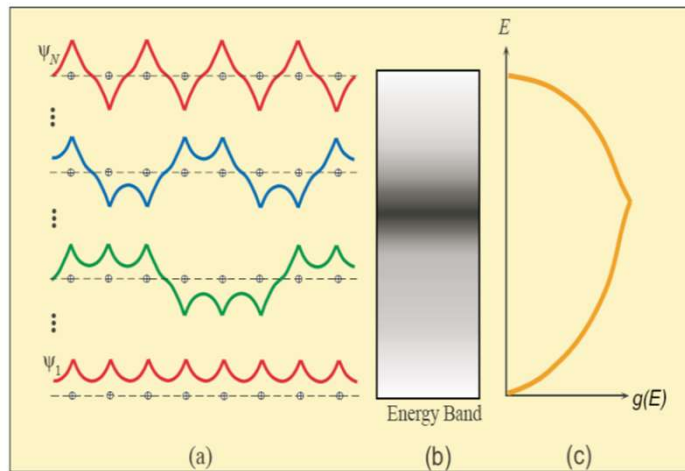
28

Table 4.2 Effective mass m_e^* of electrons in some metals

Metal	Ag	Au	Bi	Cu	K	Li	Na	Ni	Pt	Zn
$\frac{m_e^*}{m_e}$	0.99	1.10	0.047	1.01	1.12	1.28	1.2	28	13	0.85

Density of States

29



- (a) In the solid there are N atoms and N extended electron wavefunctions from ψ_1 all the way to ψ_N . There are many wavefunctions, states, that have energies that fall in the central regions of the energy band.
- (b) The distribution of states in the energy band; darker regions have a higher number of states.
- (c) Schematic representation of the density of states $g(E)$ versus energy E .

Density of States

30

$g(E)$ = Density of states

$g(E) dE$ is the number of states (*i.e.*, wavefunctions) in the energy interval E to $(E + dE)$ per unit volume of the sample.

$$g(E) = \left(8\pi 2^{1/2}\right) \left(\frac{m_e}{h^2}\right)^{3/2} E^{1/2}$$

Number of Electrons/ Volume

31

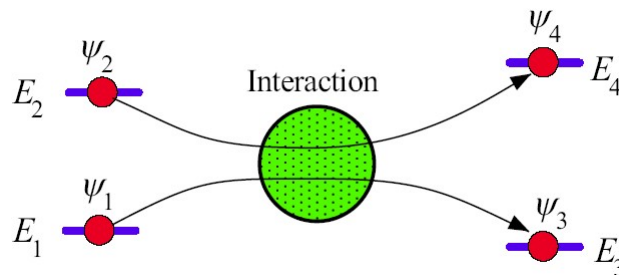
$f(E)$ = Probability that a state with energy E is occupied

$g(E)$ = Density of states

$$n = \int_{\text{Band}} f(E)g(E)dE$$

Boltzmann Classical Statistics

32



Two electrons with initial wavefunctions ψ_1 and ψ_2 at E_1 and E_2 interact and end up at different energies E_3 and E_4 . Their corresponding wavefunctions are ψ_3 and ψ_4 .

Boltzmann Classical Statistics

33

Boltzmann probability function

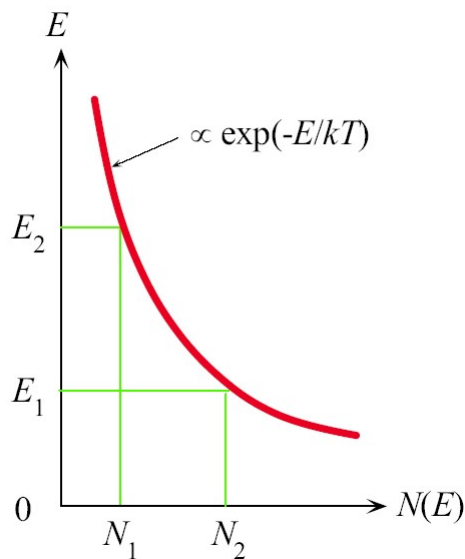
$$P(E) = A \exp\left(-\frac{E}{kT}\right)$$

Boltzmann Statistics for two energy levels

$$\frac{N_2}{N_1} = \exp\left(-\frac{E_2 - E_1}{kT}\right)$$

Boltzmann Classical Statistics

34



The Boltzmann energy distribution describes the statistics of particles, such as electrons, when there are many more available states than the number of particles.

Fermi-Dirac Statistics

35

The Fermi-Dirac function

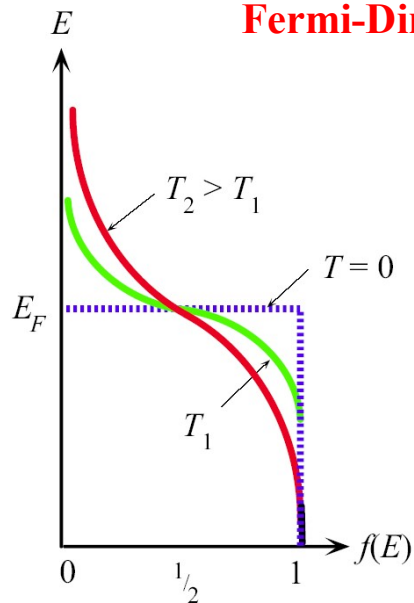
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

where E_F is a constant called the **Fermi energy**.

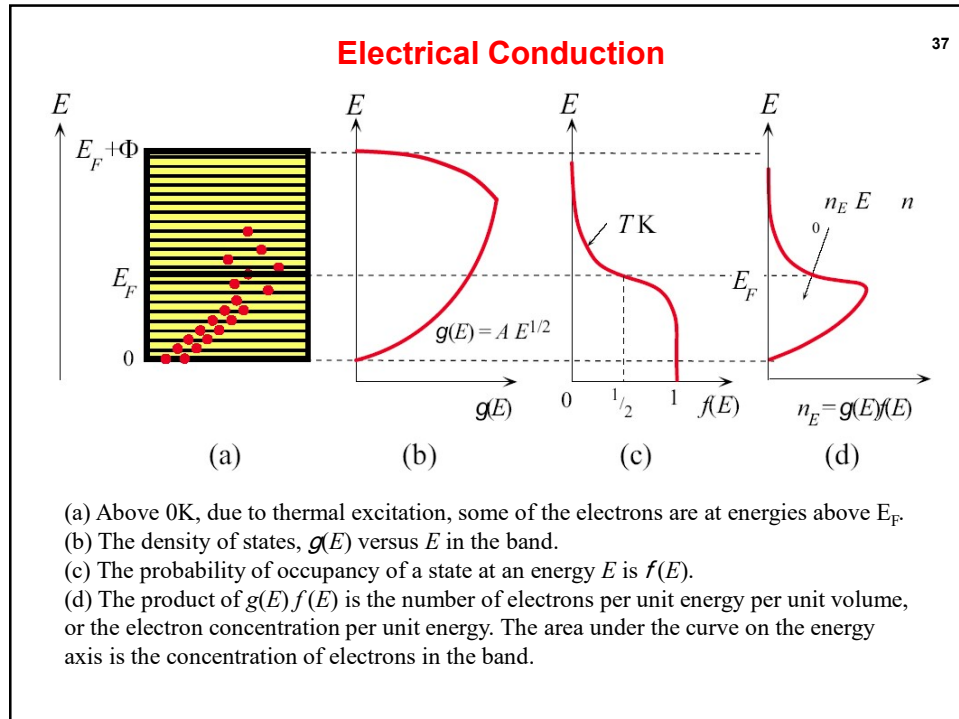
$f(E)$ = the probability of finding an electron in a state with energy E is given

Fermi-Dirac Statistics

36



The fermi-Dirac $f(E)$ describes the statistics of electrons in a solid. The electrons interact with each other and the environment, obeying the Pauli exclusion principle.



Fermi Energy 38

Fermi energy at $T = 0$ K

$$E_{FO} = \left(\frac{h^2}{8m_e} \right) \left(\frac{3n}{\pi} \right)^{2/3}$$

n is the concentration of conduction electrons (free carrier concentration)

Fermi energy at T (K)

$$E_F(T) = E_{FO} \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{E_{FO}} \right)^2 \right]$$

Average energy per electron

39

Average energy per electron at 0 K

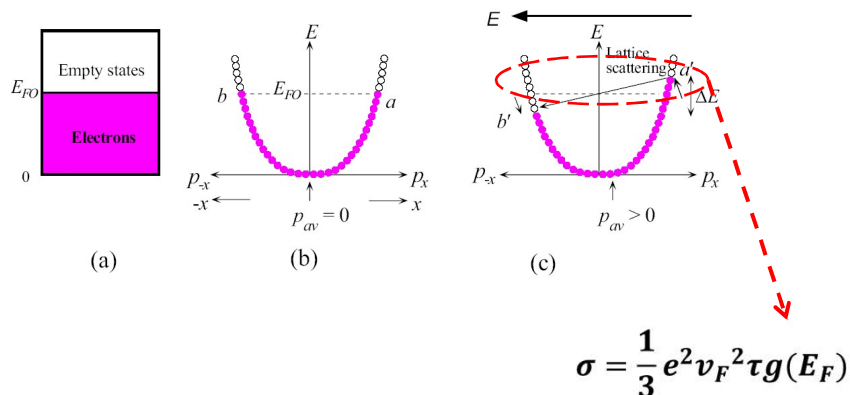
$$E_{\text{av}}(0) = \frac{3}{5} E_{FO}$$

Average energy per electron at T (K)

$$E_{\text{av}}(T) = \frac{3}{5} E_{FO} \left[1 + \frac{5\pi^2}{12} \left(\frac{kT}{E_{FO}} \right)^2 \right]$$

Conduction in Metals

40



Effect of $g(E_F)$: Cu and Mg

Effect of τ : Ni – 3d and 4s bands

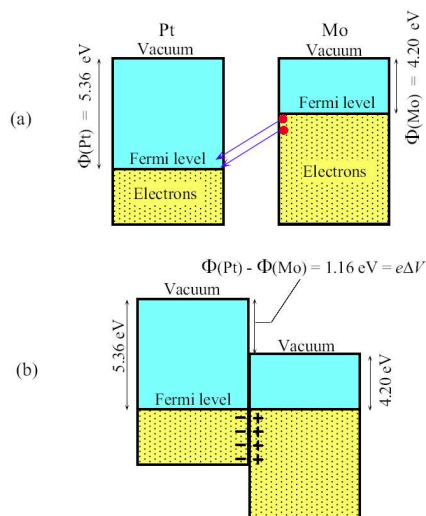
Fermi Energy Significance

41

For a given metal the Fermi energy represents the free energy per electron called the **electrochemical potential**. The Fermi energy is a measure of the potential of an electron to do electrical work ($e \times V$) or nonmechanical work, through chemical or physical processes.

Metal-Metal Contact: Contact potential

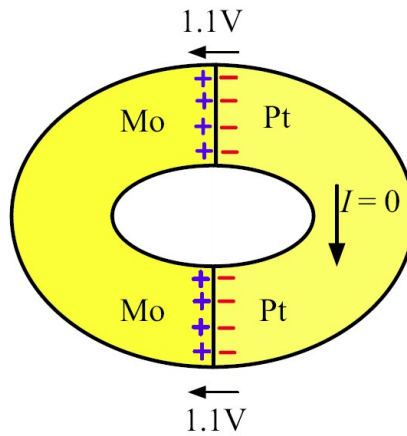
42



- (a) Electrons are more energetic in Mo, so they tunnel to the surface of Pt.
- (b) Equilibrium is reached when the Fermi levels are lined up.
When two metals are brought together, there is a contact potential ΔV .

Metal-Metal Contact: Contact potential

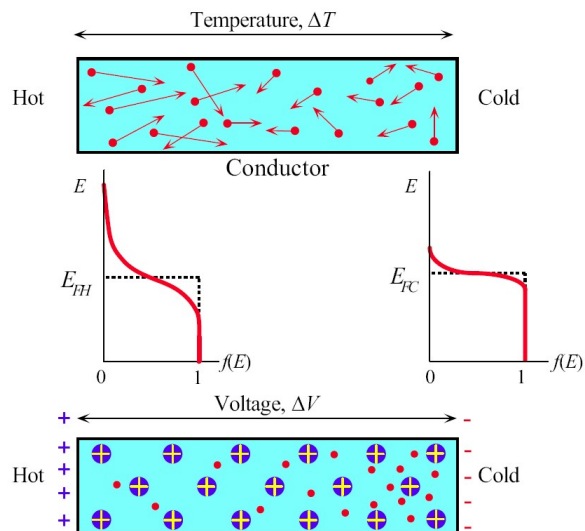
43



There is no current when a closed circuit is formed by two different metals, even though there is a contact potential at each contact.
The contact potentials oppose each other.

Seebeck Effect

44



The Seebeck effect. A temperature gradient along a conductor gives rise to a potential difference.

Seebeck Effect

45

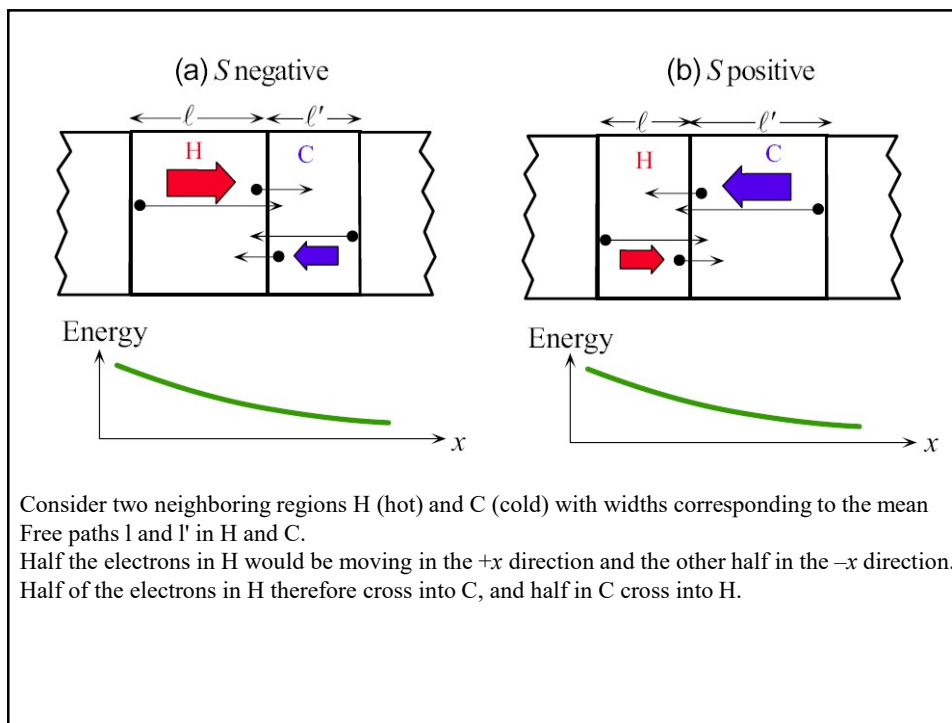
Seebeck effect (thermoelectric power)

is the built-in potential difference ΔV across a material due to a temperature difference ΔT across it.

$$S = \frac{\Delta V}{\Delta T}$$

Sign of S

is the potential of the cold side with respect to the hot side; negative if electrons have accumulated in the cold side.



Seebeck coefficient for metals

47

$$S \approx - \frac{\pi^2 k^2 T}{3eE_{FO}} x$$

Mott and Jones thermoelectric power equation

x = a numerical constant that takes into account how various charge transport parameters, such as the mean free path ℓ , depend on the electron energy.

x values are tabulated in Table 4.3

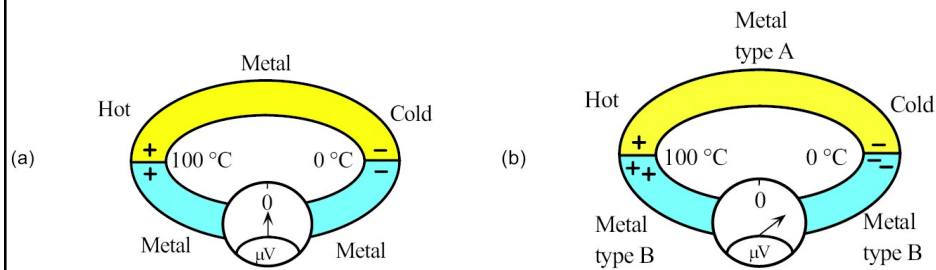
DOES NOT APPLY TO MATERIALS HAVING OVERLAPPING BANDS –
e.g. Ni

48

Table 4.3 Seebeck coefficients of selected metals (from various sources)

Metal	S at 0 °C ($\mu\text{V K}^{-1}$)	S at 27 °C ($\mu\text{V K}^{-1}$)	E_F (eV)	x
Al	−1.6	−1.8	11.6	2.78
Au	+1.79	+1.94	5.5	−1.48
Cu	+1.70	+1.84	7.0	−1.79
K		−12.5	2.0	3.8
Li	+14		4.7	−9.7
Mg	−1.3		7.1	1.38
Na		−5	3.1	2.2
Pd	−9.00	−9.99		
Pt	−4.45	−5.28		

49



- (a) If Al wires are used to measure the Seebeck voltage across the Al rod, then the net emf is zero.
- (b) The Al and Ni have different Seebeck coefficients. There is therefore a net emf in the Al-Ni Circuit between the hot and cold ends that can be measured.

50

Thermocouple

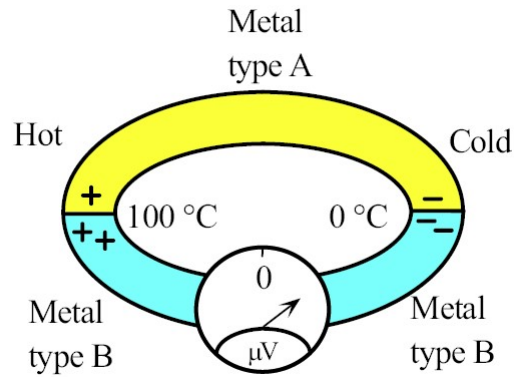
We can only measure differences between thermoelectric powers of materials.

When two different metals A and B are connected to make a **thermocouple**, then the net EMF is the voltage difference between the two elements.

$$V_{AB} = \int_{T_o}^T (S_A - S_B) dT = \int_{T_o}^T S_{AB} dT$$

Thermocouple Equation

51



$$V_{AB} = a\Delta T + b(\Delta T)^2$$

52

Table 4.4 Thermoelectric emf for metals at 100 and 200 °C with respect to Pt and the reference junction at 0 °C

Material	emf (mV)	
	At 100 °C	At 200 °C
Copper, Cu	0.76	1.83
Aluminum, Al	0.42	1.06
Nickel, Ni	−1.48	−3.10
Palladium, Pd	−0.57	−1.23
Platinum, Pt	0	0
Silver, Ag	0.74	1.77
Alumel	−1.29	−2.17
Chromel	2.81	5.96
Constantan	−3.51	−7.45
Iron, Fe	1.89	3.54
90% Pt–10% Rh (platinum-rhodium)	0.643	1.44



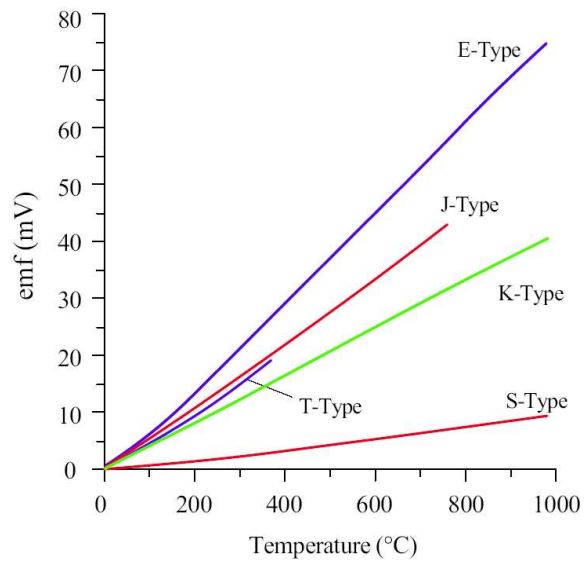
53



Thermocouples are widely used to measure the temperature.

LEFT: A thermocouple pair embedded in a stainless steel sheath-probe. The thermocouple junction inside the probe is in thermal contact with the probe tip, and, electrically insulated from the probe metal.

[SOURCE: Courtesy of Omega]



54

Output emf versus temperature (°C) for various thermocouple between 0 and 1000 °C

Examples of vacuum tubes using thermionic emission

55



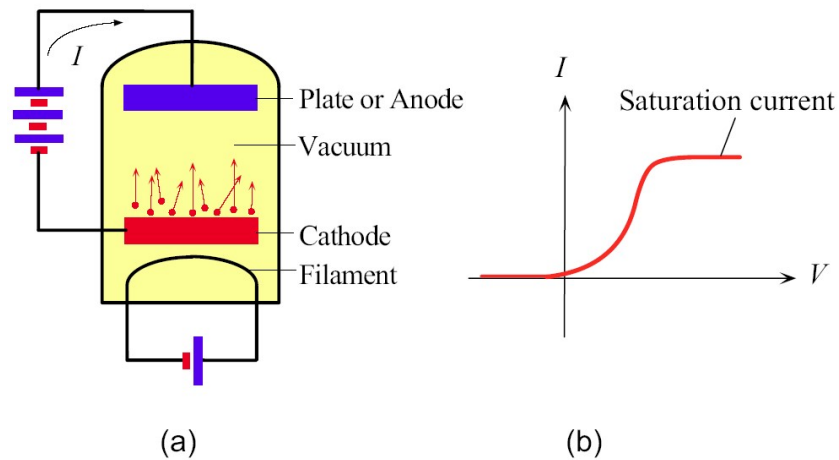
TOP: UHF Tetrode vacuum tubes that can handle up to 30 kW, and provide gains up to 17 dB

[SOURCE: Courtesy of Thales]

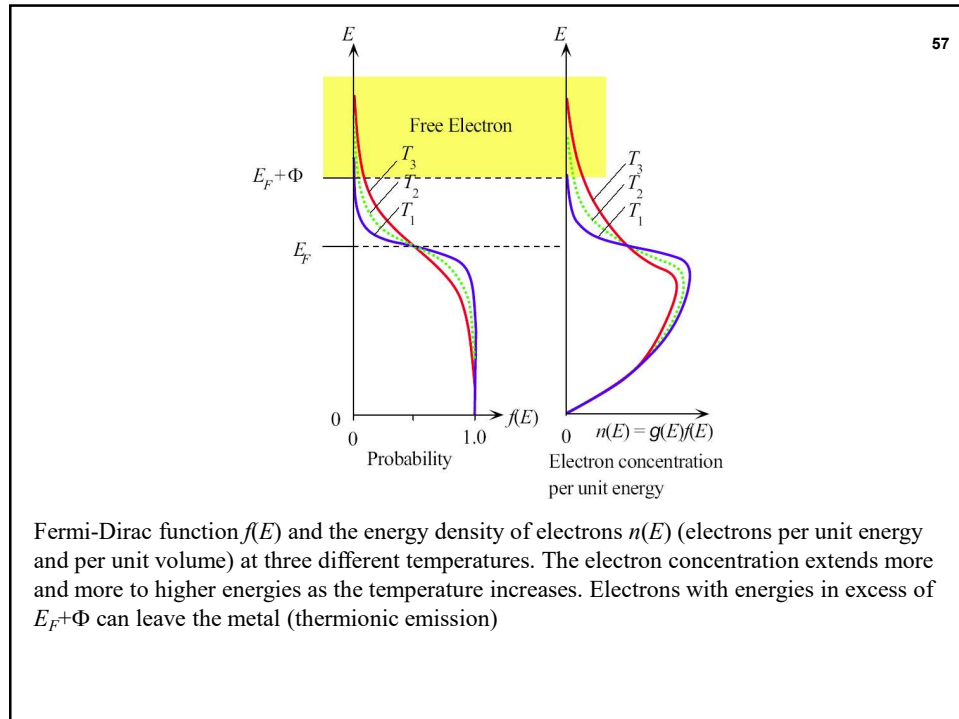


LEFT: Klystrons are used as the final amplifier stage in many UHF television transmitters.

[SOURCE: Courtesy of Thales]



56



58

Thermionic Emission

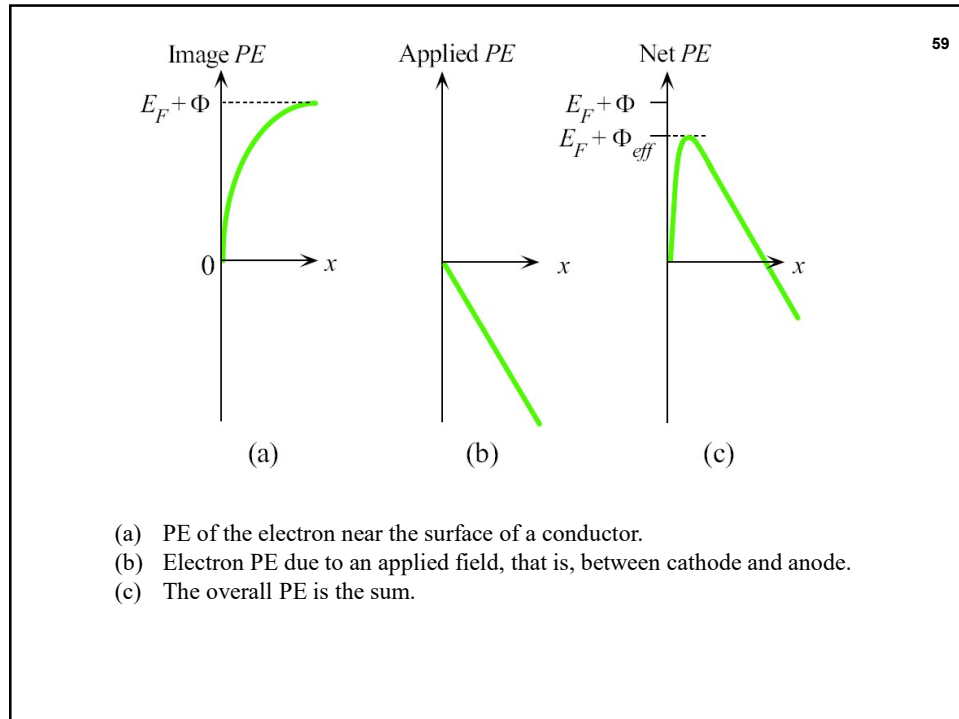
Richardson-Dushman thermionic emission equation

$$J = B_o T^2 \exp\left(-\frac{\Phi}{kT}\right)$$

$B_o = 4\pi m_e k^2 / h^3 = 120 \times 10^6 \text{ A m}^{-2} \text{ K}^{-2}$
Richardson-Dushman constant

$$J = B_e T^2 \exp\left(-\frac{\Phi}{kT}\right)$$

where B_e = effective emission constant = $(1-R) B_o$
R = Reflection coefficient



Schottky effect

60

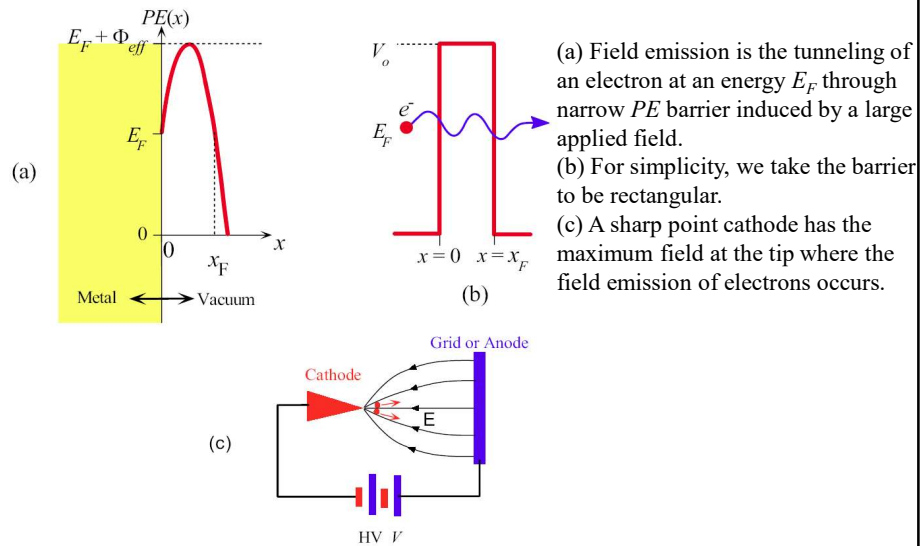
When a positive voltage is applied to the anode with respect to the cathode, the electric field at the cathode helps the thermionic emission process by lowering the *PE* barrier Φ by an amount $\beta_s \mathcal{E}^{1/2}$. The current density in field assisted thermionic emission is

Metal's work function Schottky coefficient

$$J = B_e T^2 \exp \left(- \frac{\Phi - \beta_s \mathcal{E}^{1/2}}{kT} \right)$$

Field assisted emission is field assisted tunneling from the cathode

61



Field-assisted Tunneling

62

Field-assisted tunneling probability

Effective work function due to the Schottky effect

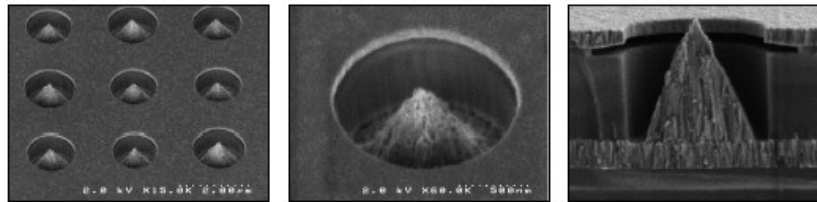
$$p \approx \exp \left[- \frac{2(2m_e \Phi_{\text{eff}})^{1/2} \Phi}{e\hbar E} \right]$$

Field-assisted tunneling: the Fowler-Nordheim equation

$$J_{\text{field-emission}} \approx C E^2 \exp \left(- \frac{\mathcal{E}_c}{E} \right)$$

Applied field at the cathode

63



Left: A scanning electron microscope image of an array of electron field emitters (icebergs). Center: One iceberg. Right: A cross section of a field emitter. Each iceberg is a source of electron emission arising from Fowler–Nordheim field emission; for further information see B. Chalamala, et al., *IEEE Spectrum*, April 1998, pp. 42–51.

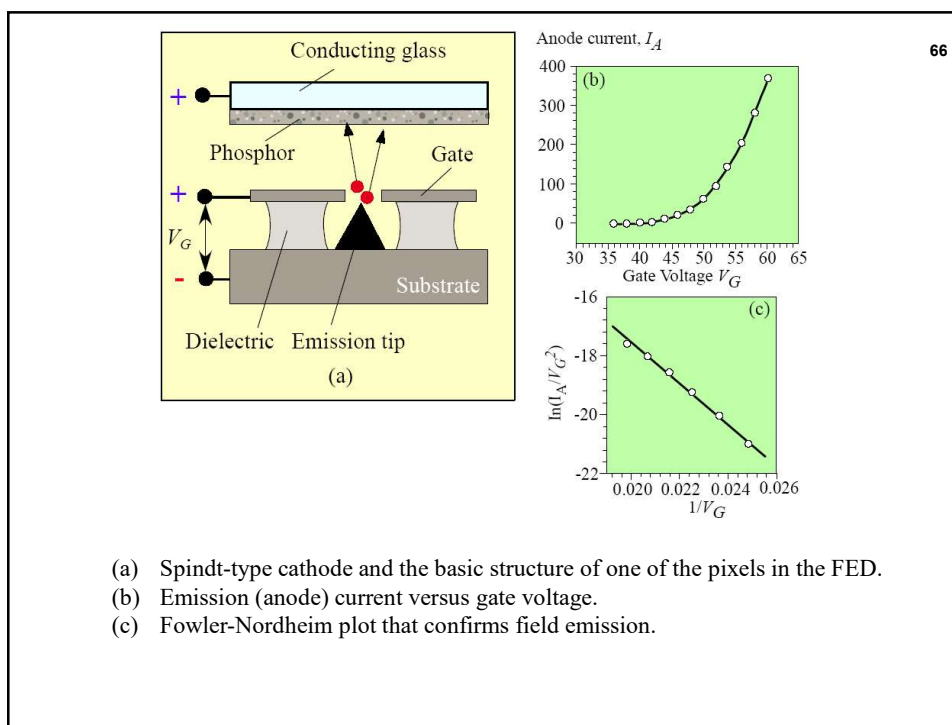
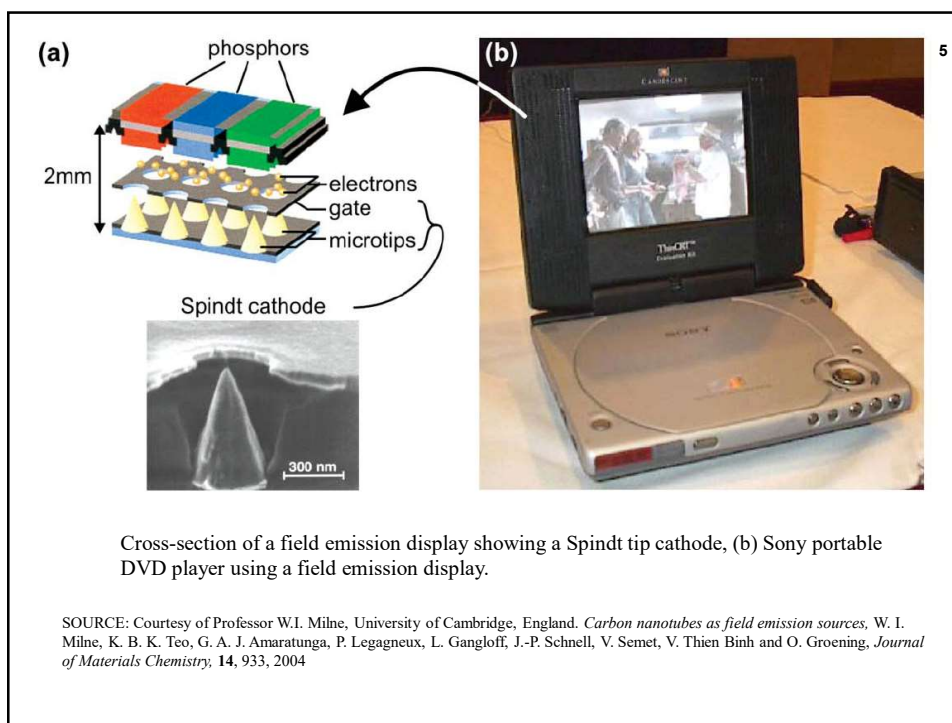
| SOURCE: Courtesy of Dr. Babu Chalamala, Flat Panel Display Division, Motorola.

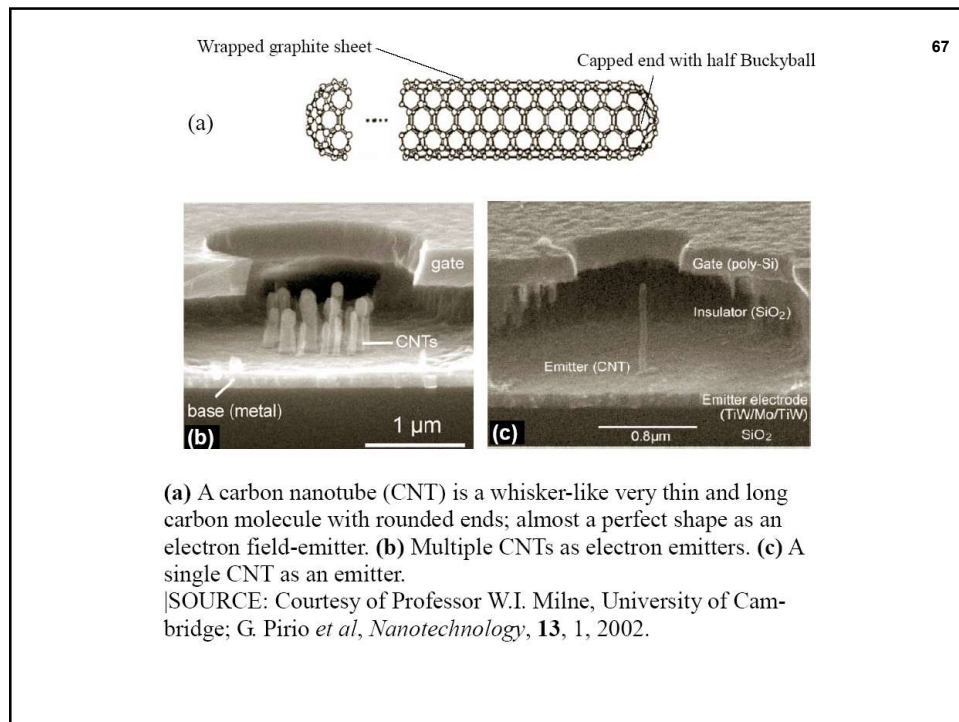
64



Motorola's prototype flat panel display based on the Fowler-Nordheim field emission principle. The display is 14 cm in diagonal and 3.5 mm thick with a viewing angle 160°. Each pixel (325 μm thick) uses field emission of electrons from microscopic sharp point sources (icebergs). Emitted electrons impinge on colored phosphors on a screen and cause light emission by cathodoluminescence. There are millions of these microscopic field emitters to constitute the image.

| SOURCE: Courtesy of Dr. Babu Chalamala, Flat Panel Display Division, Motorola.





CNT (Carbon NanoTube)

68

A carbon nanotube (CNT) is a very thin filament-like carbon molecule whose diameter is in the nanometer range but whose length can be quite long, e.g., 10-100 microns, depending on how it is grown or prepared.