ECE 340: Semiconductor Electronics

Chapter 3: Energy bands and charge carriers in semiconductors (part I)

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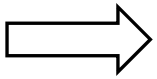
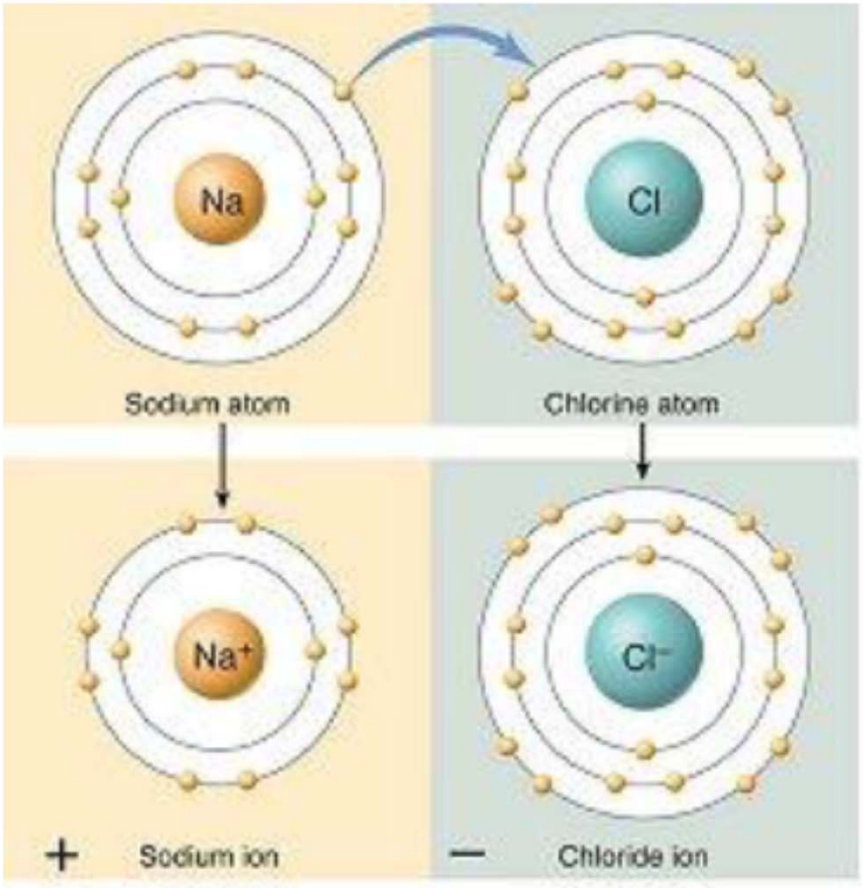
Outline

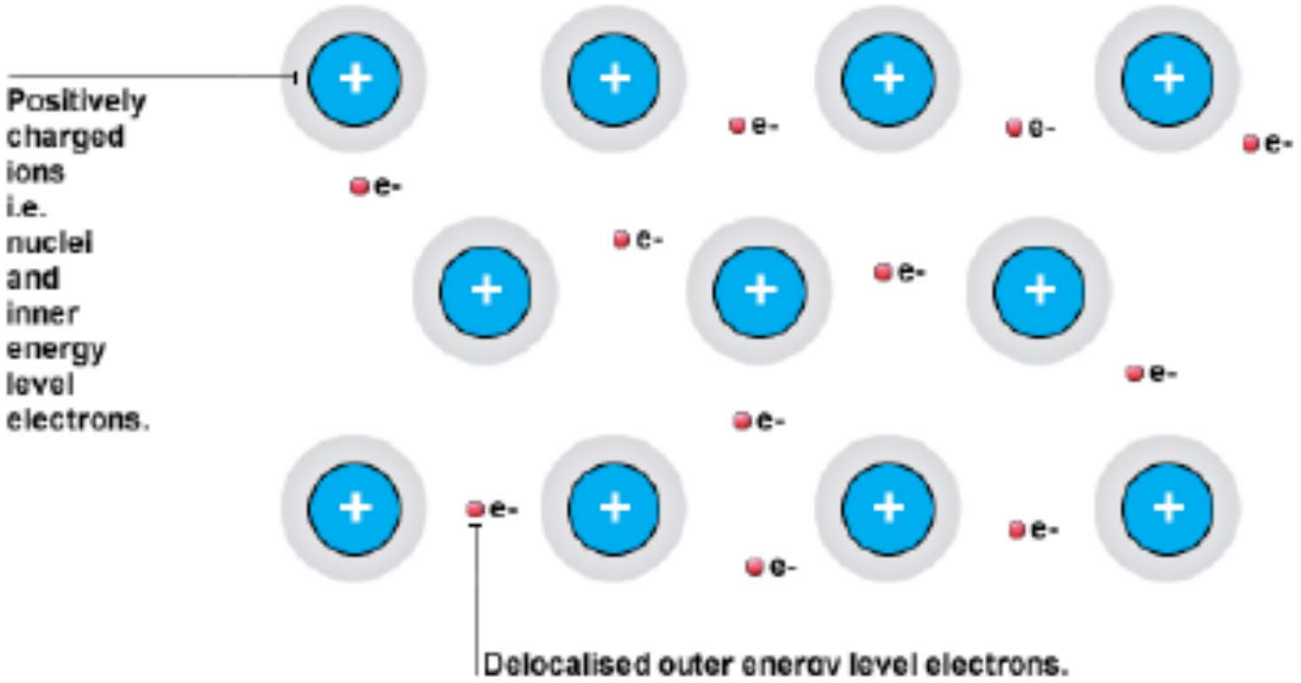


- Bonding force and energy band
  - Bonding forces in solids
  - Energy bands
  - Metals, semiconductors, and insulators
  - Direct and indirect semiconductors
- Charge carriers in semiconductors
  - Electrons and holes
  - Effective mass
  - Intrinsic material
  - Extrinsic material

Ionic bonding of NaCl (insulator)

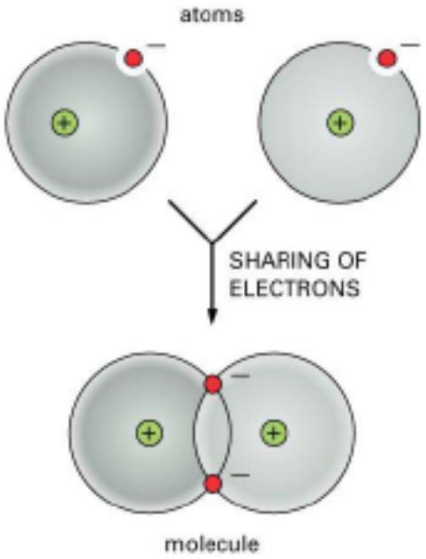


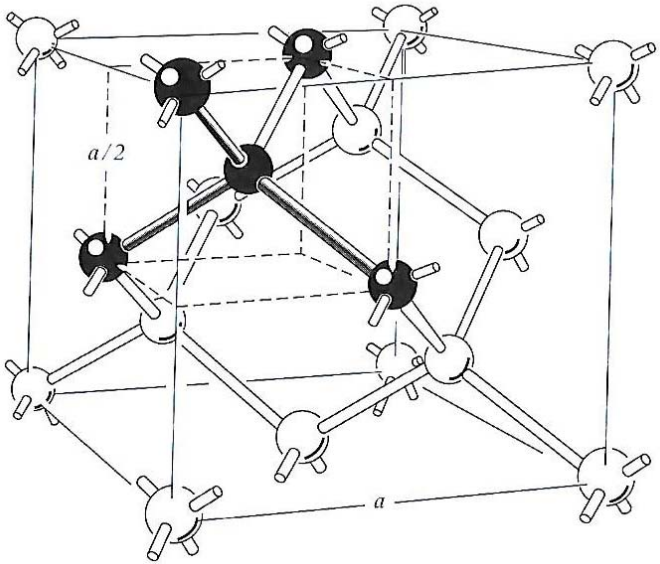
Metallic Bonding

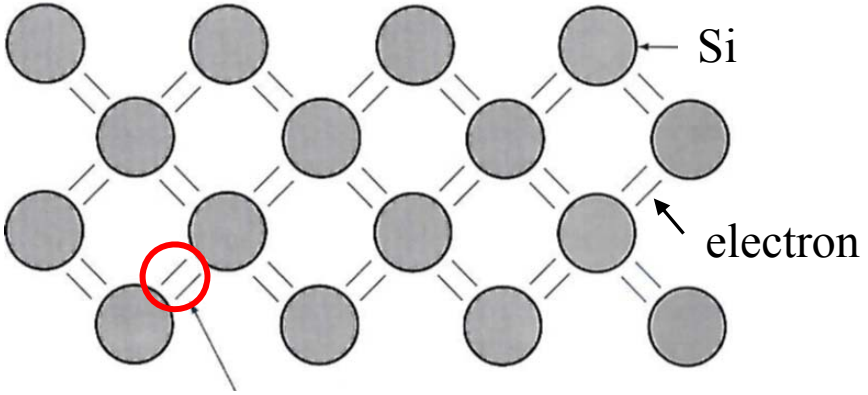


- Outer shell is only partially filled.
- Screening by other charges makes the valence electron very loosely bound.
- Outer electron contributed to crystal as a whole.
- Bonding can be very complex depending on the compound involved.

Covalence bonding in silicon crystal







Two electrons per bond

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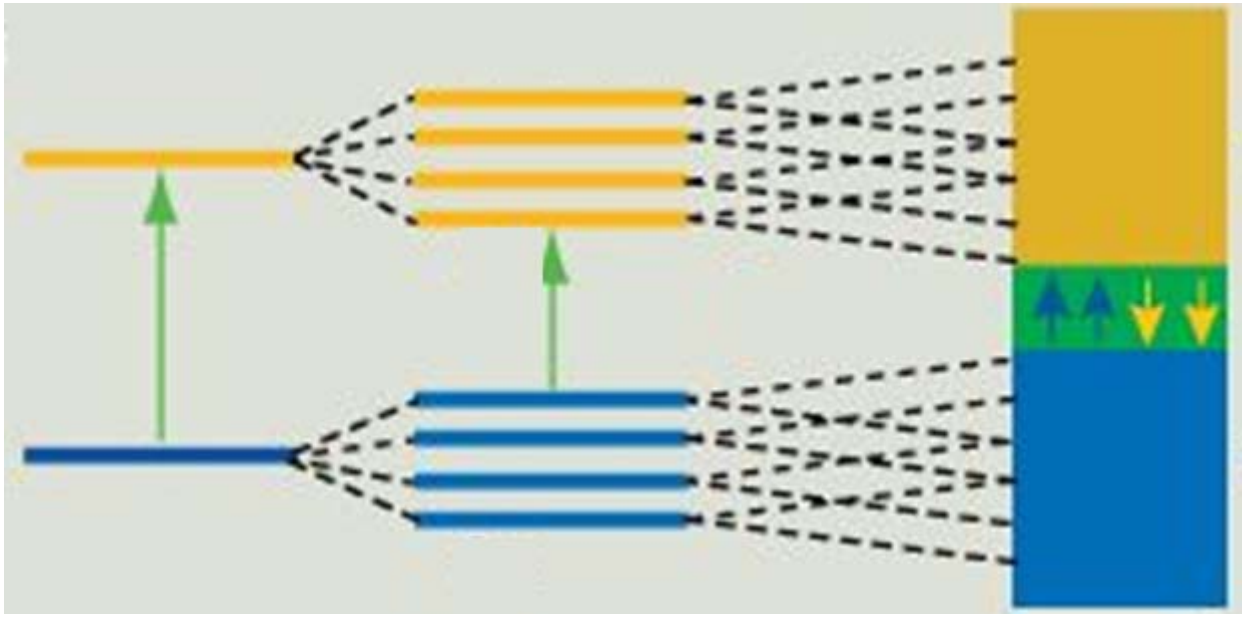
Energy Levels vs Energy Bands

- Isolated atoms: no overlap of electronic wave functions, only has original discrete energy levels;
- Interacting atoms: overlaps of electronic wave functions, many new energy levels are created through hybridization. If you have too many levels, you get a band!

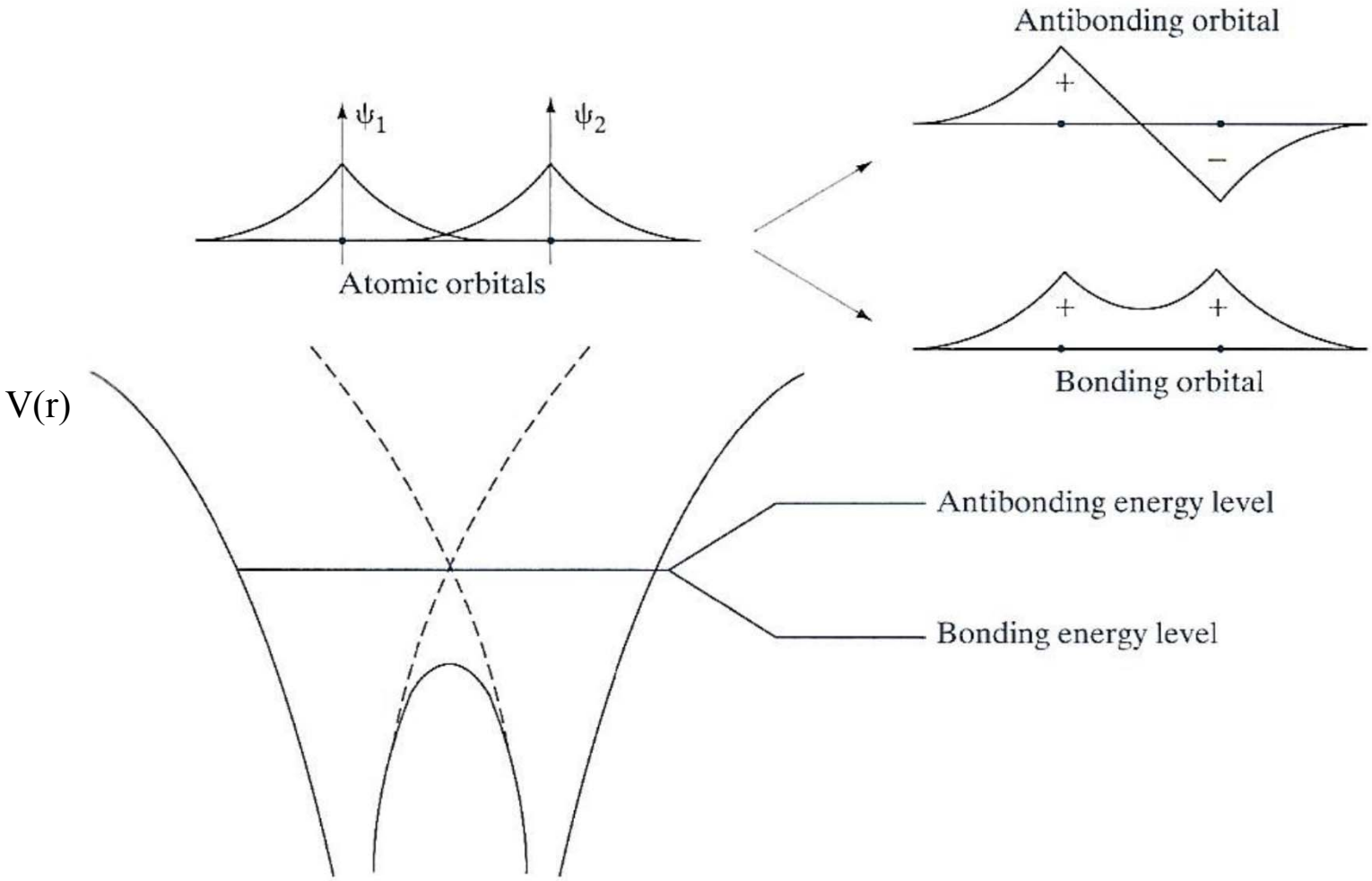


Single atom

4 atoms in close proximity

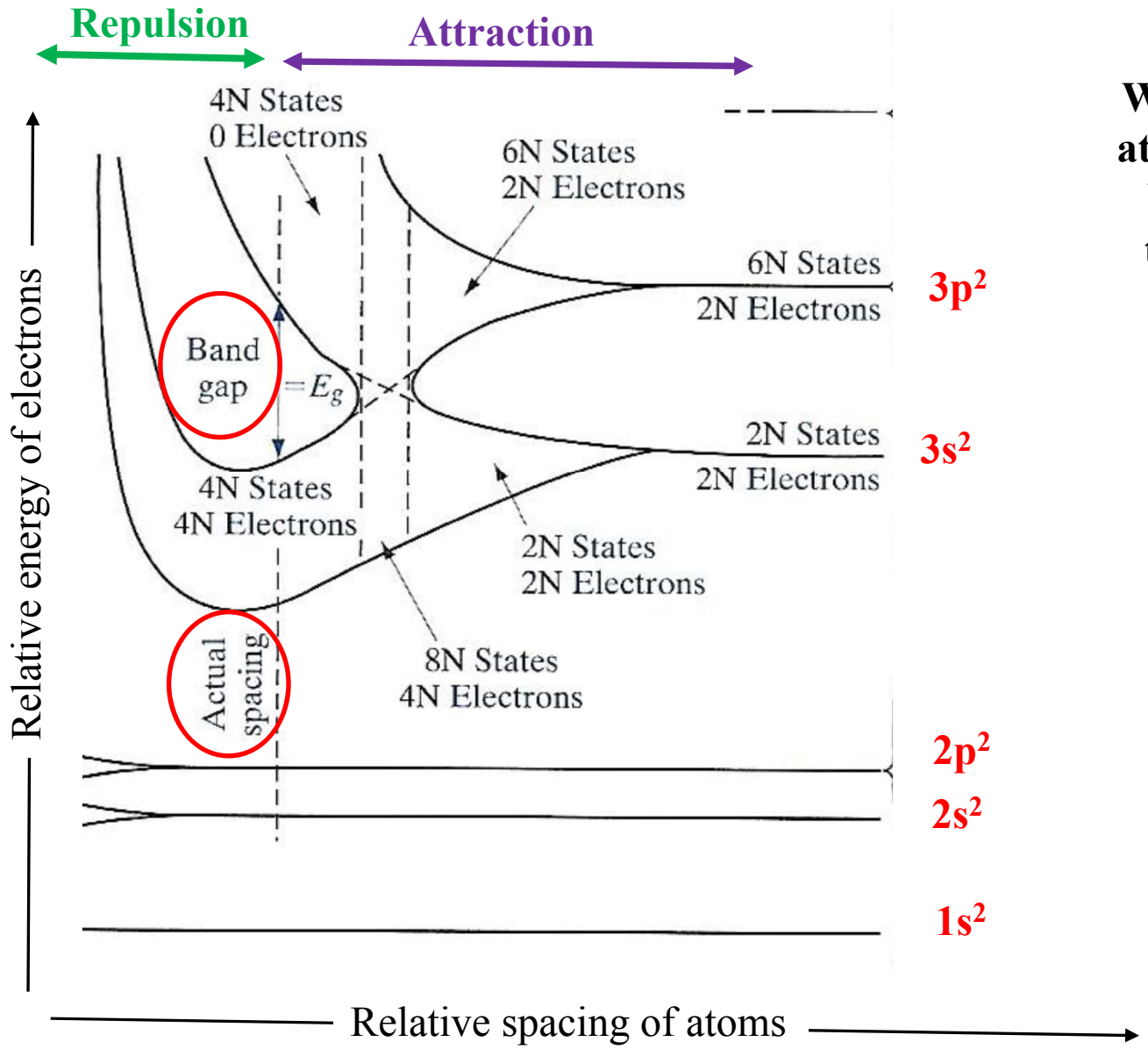
Multitudes of atoms in close proximity

Bring two silicon atoms together



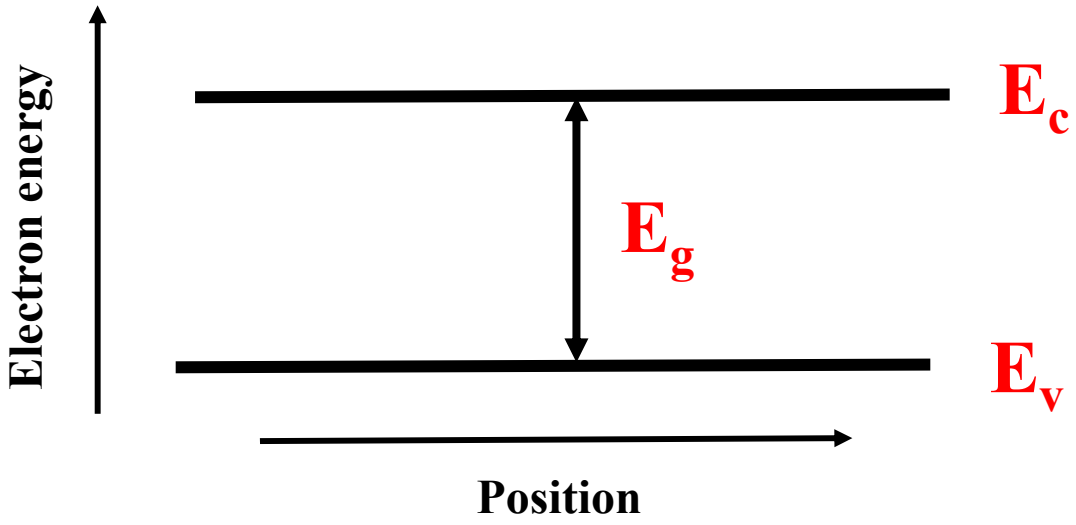
Leads to two distinct "normal" modes – a higher energy antibonding orbital and a lower energy bonding orbital. The electron probability density is higher in the region between the ion cores, leading to lowering of the bonding energy

Energy levels in Si as a function of interatomic spacing



When N Si atoms were brought together

Energy Band Diagram



Simplified version of energy band model, indicating:

- Bottom edge of the conduction band (E_c)
- Top edge of the valence band (E_v)

Ec and Ev are separated by the **band gap energy** E_g

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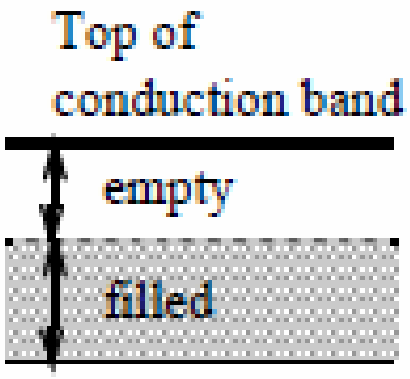
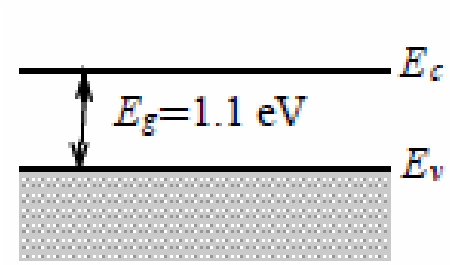
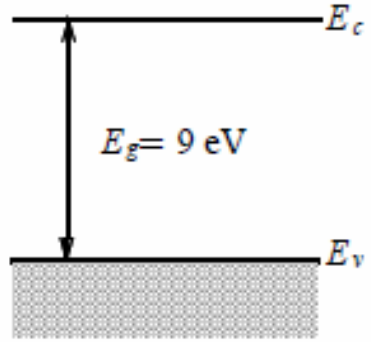
Metal, semiconductor and insulator



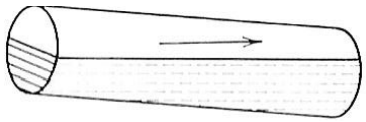
Metal

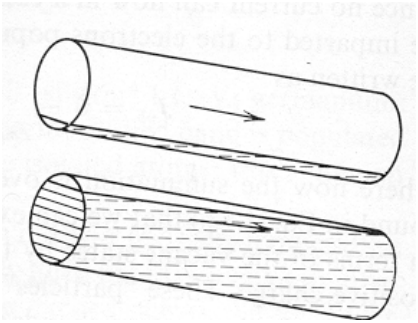


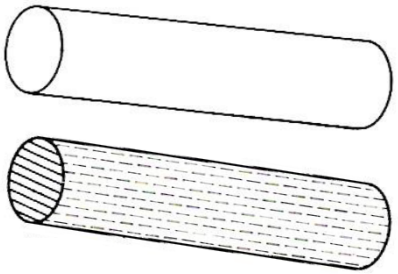
Si, Semiconductor



SiO_2, insulator

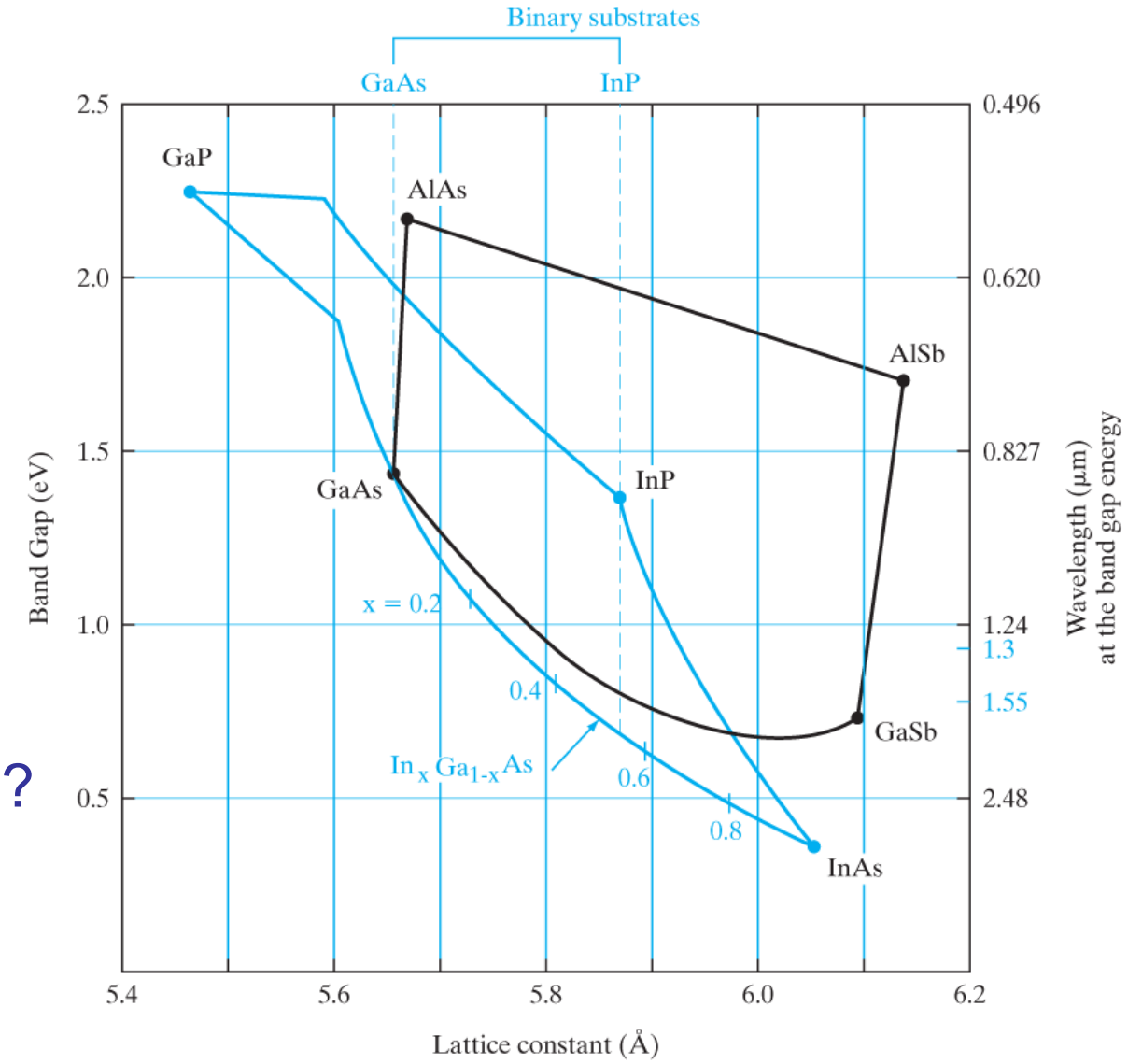






- Band structure explains why SiO_2 (diamond, etc) is insulating, silicon is semiconducting, copper is a metal
- *For electrons to be accelerated in an electric field they must be able to move into new, unoccupied energy states.*

- How do band gaps vary with lattice size? (is there a trend?)



- How do band gaps vary with temperature?

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E-k diagram

E: energy

k: wavevector, or propagation constant $k = 2\pi/\lambda$

momentum $p = \hbar k$

- For classic objects, the kinetic energy $E_{kE} = \frac{mV^2}{2} = \frac{P^2}{2m} = \frac{\hbar^2 k^2}{2m}$

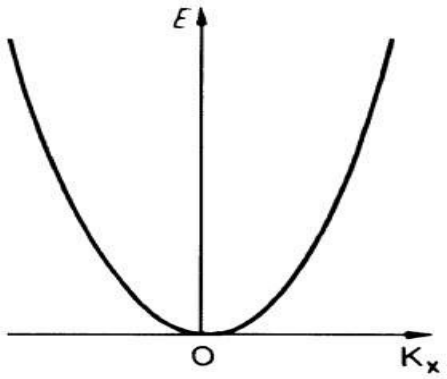
  E~k curve (dispersion curve) is a "parabola".

- In quantum mechanics, free electron has the planewave wavefunction,

$$\psi_k(x) = e^{j\boldsymbol{k}_x \cdot \boldsymbol{x}}$$

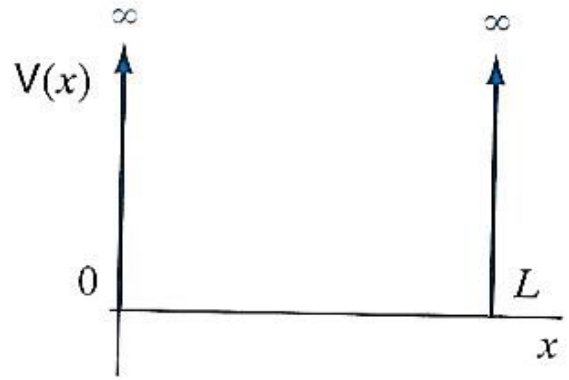
the E~k relationship is similar:

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



E-k diagram

For particle in a box:

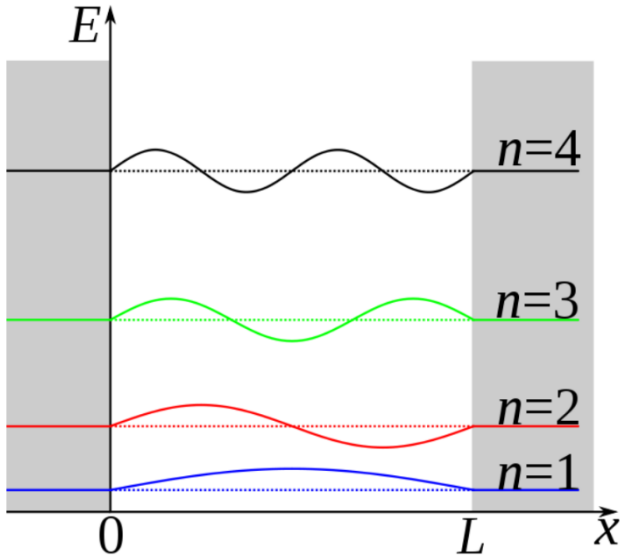


$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

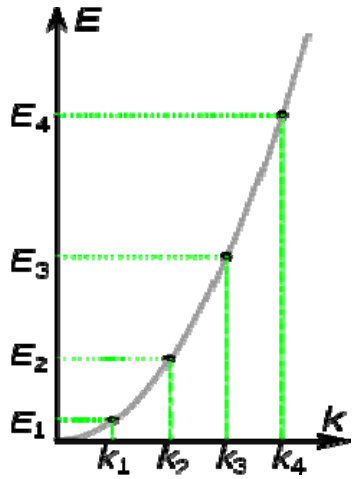
$$\Rightarrow \quad \psi_n = \sqrt{\frac{2}{L}}\sin(kx)$$

$$\mathrm{k} = \frac{n\pi}{L}, \qquad n = 1,2,3,\ldots$$

$$\mathrm{E} = \frac{n^2\pi^2\hbar^2}{2mL^2}, \qquad n = 1,2,3,\ldots$$



$$\Rightarrow \quad E = \frac{\hbar^2 k^2}{2m}$$

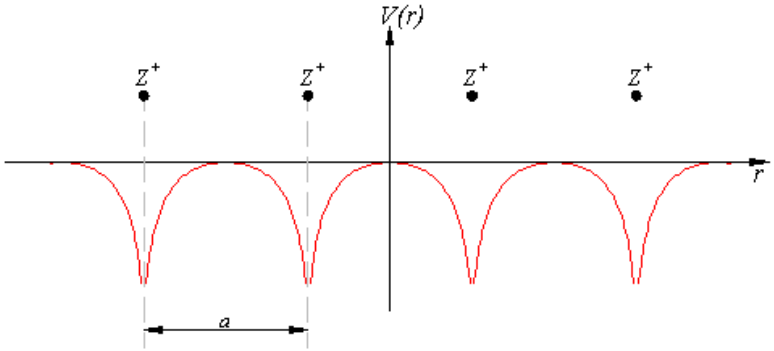


E~K relation in periodical lattice

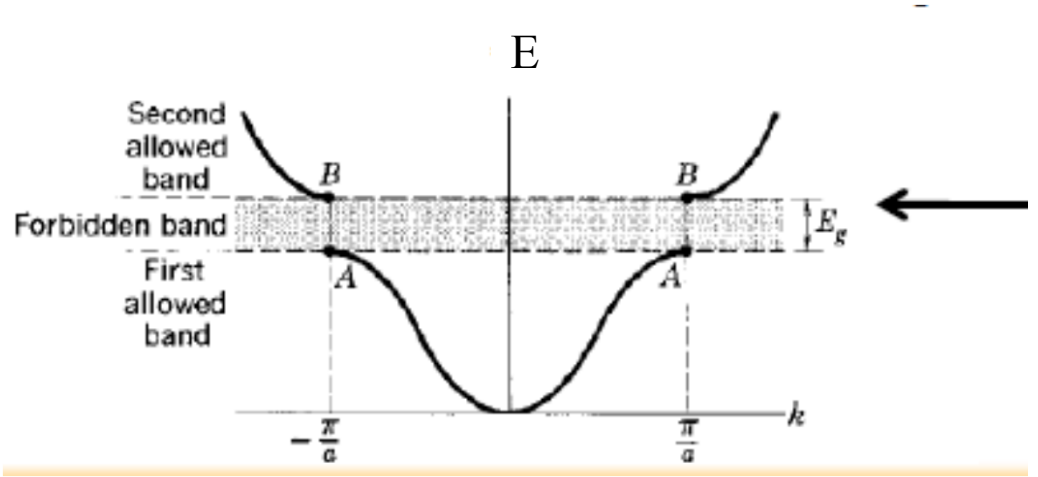
For electron in a periodic lattice, i.e a periodic Col potential, the solution of the Schrödinger equation wavefunction is in a form:

$$\psi_k(x) = U(k_x, \mathrm{x})e^{j\boldsymbol{k}_x \cdot \boldsymbol{x}}$$

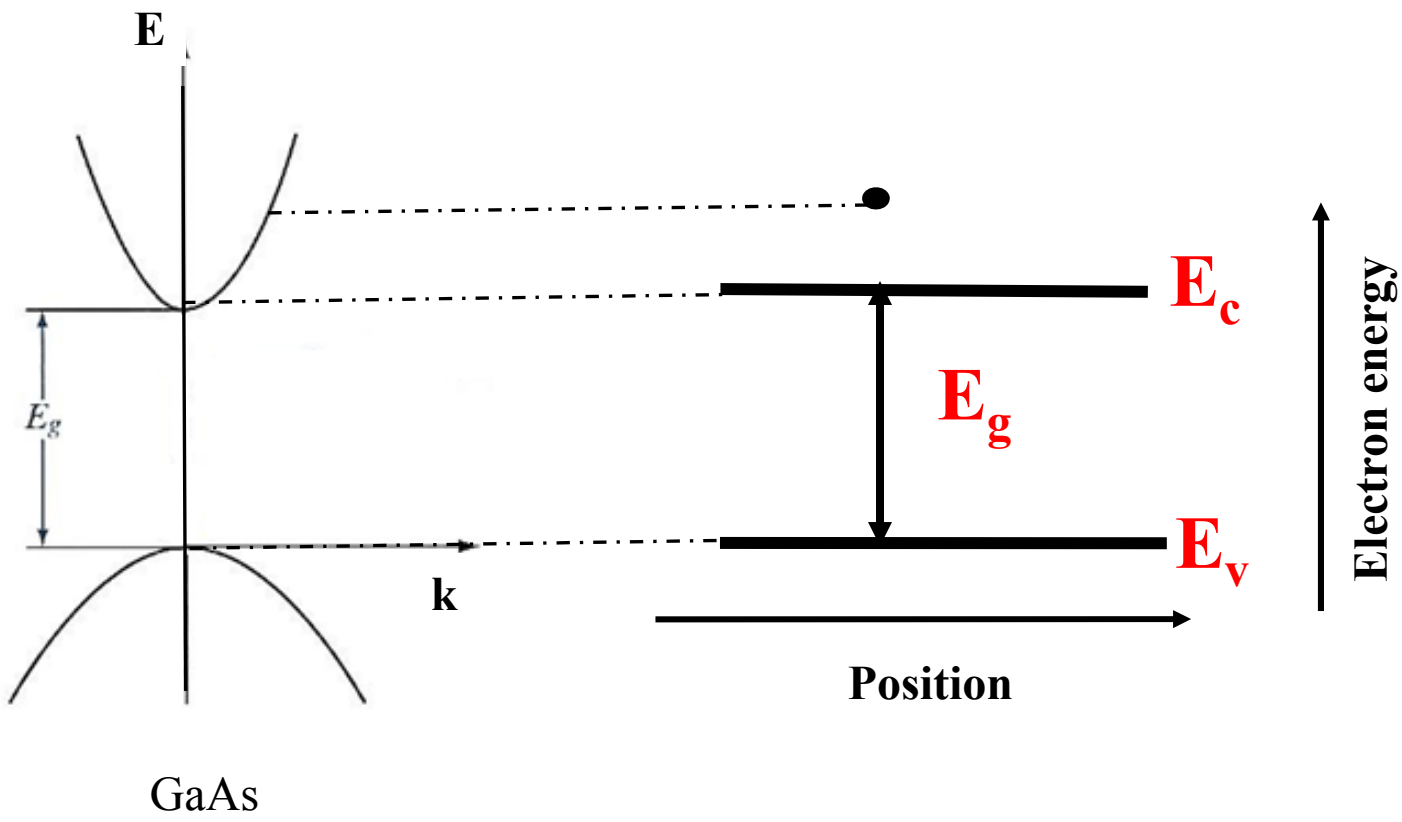
(called Bloch function).



E~k relation is periodic with a bandgap. It is parabolic near the minimum or maximum of a band.

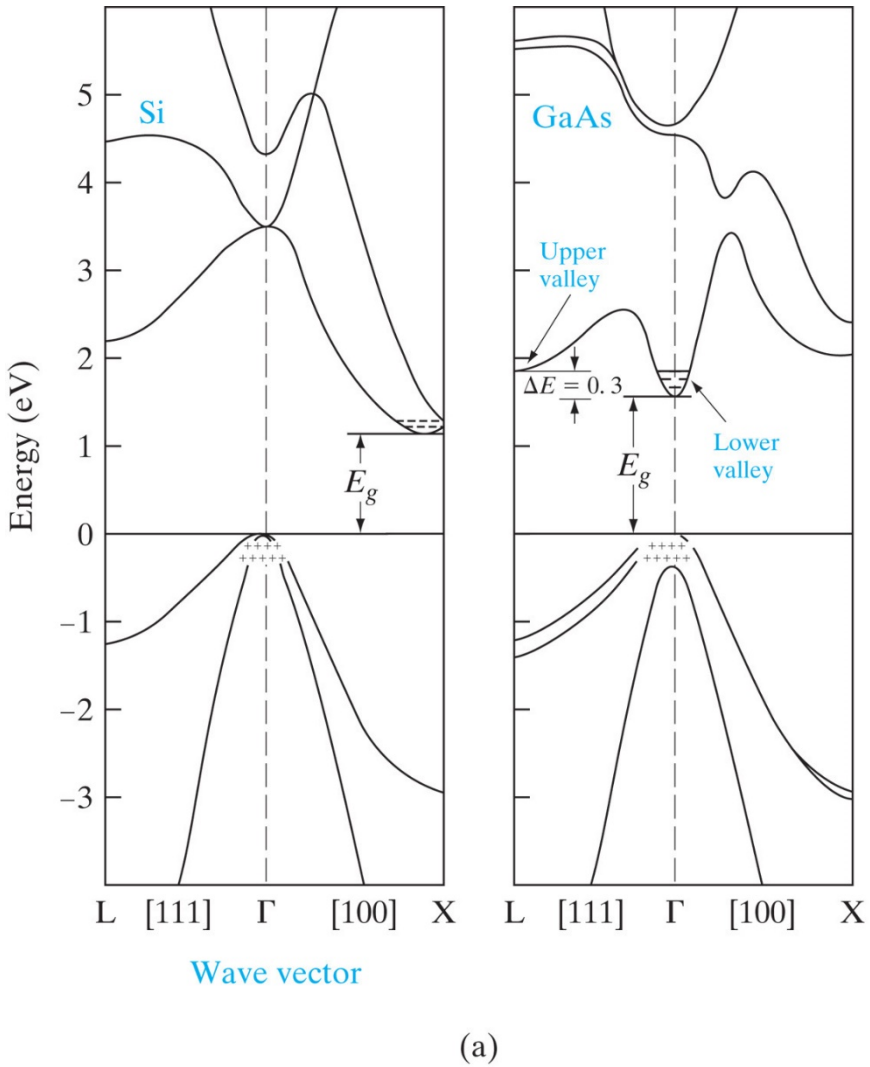


E-K vs. E-X

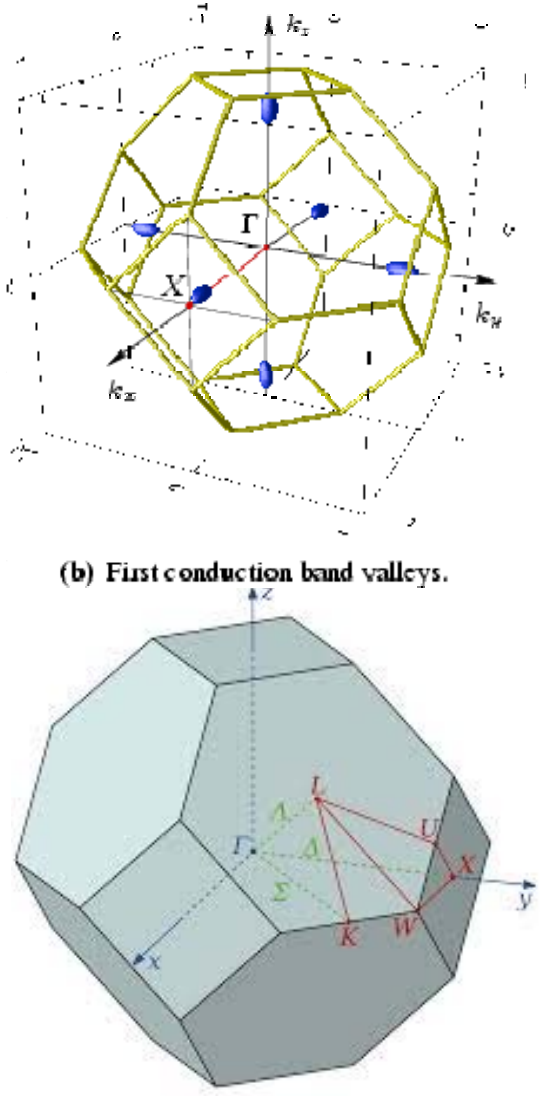


GaAs

Band structures in semiconductors



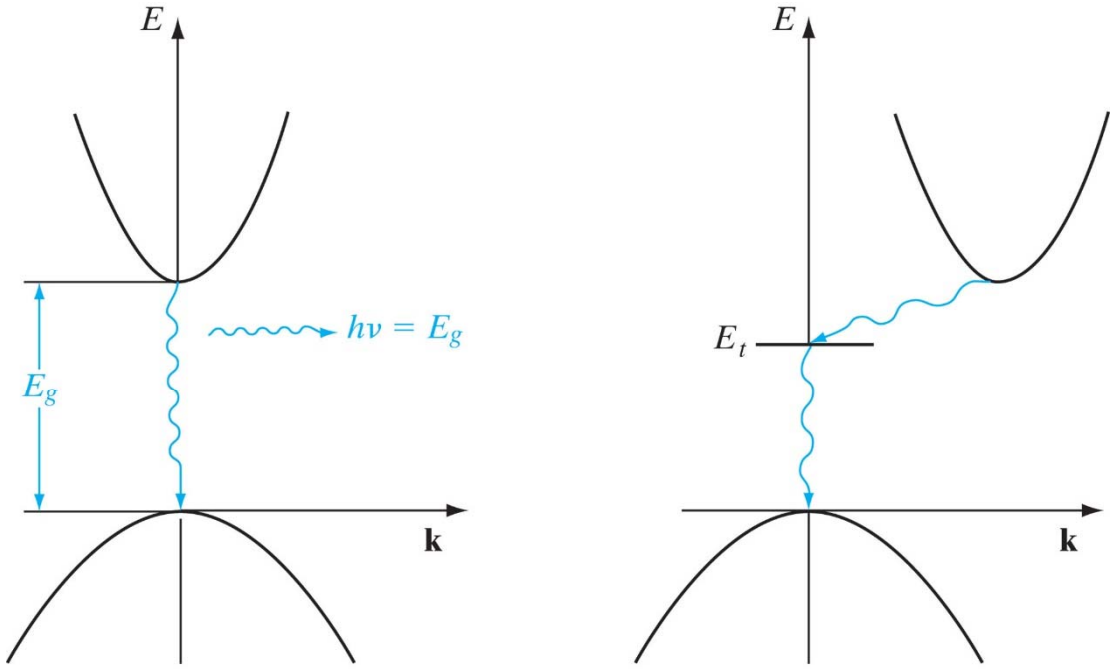
(a)



(b) First conduction band valleys.

Direct and indirect band gap

Direct band gap **Indirect band gap**



(a) Direct (b) Indirect

Direct band gap: minimum in the conduction band and maximum of valence band occurs at the **same** k value.

Indirect band gap: minimum in the conduction band and maximum of valence band occurs at the **different** k value

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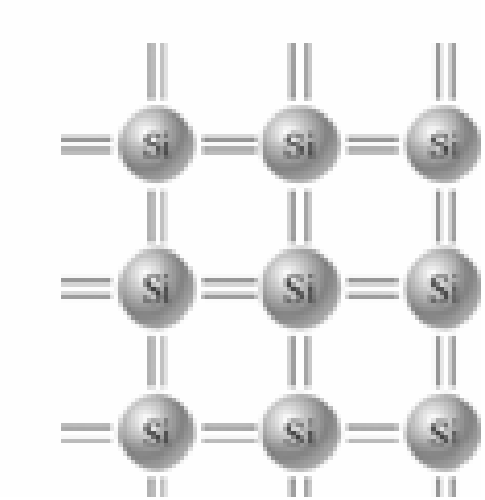
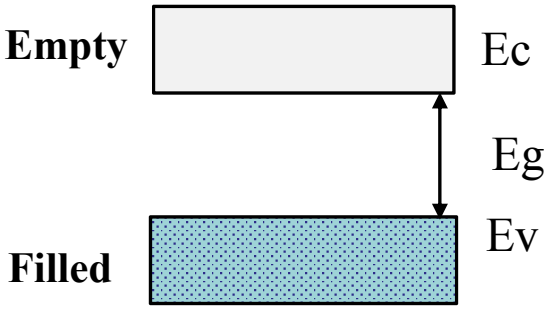
Electron and holes

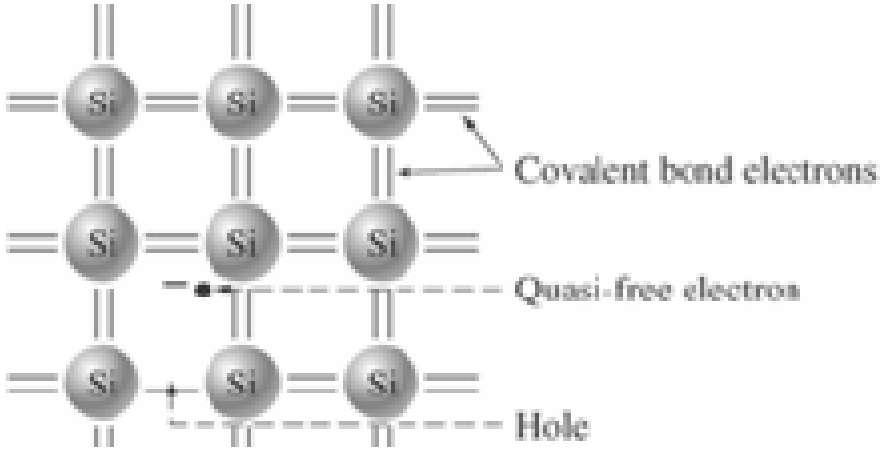
T=0K

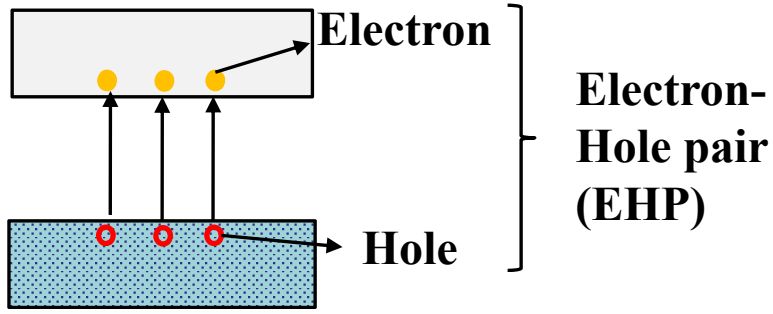




No free electrons in the semiconductor

T>0K



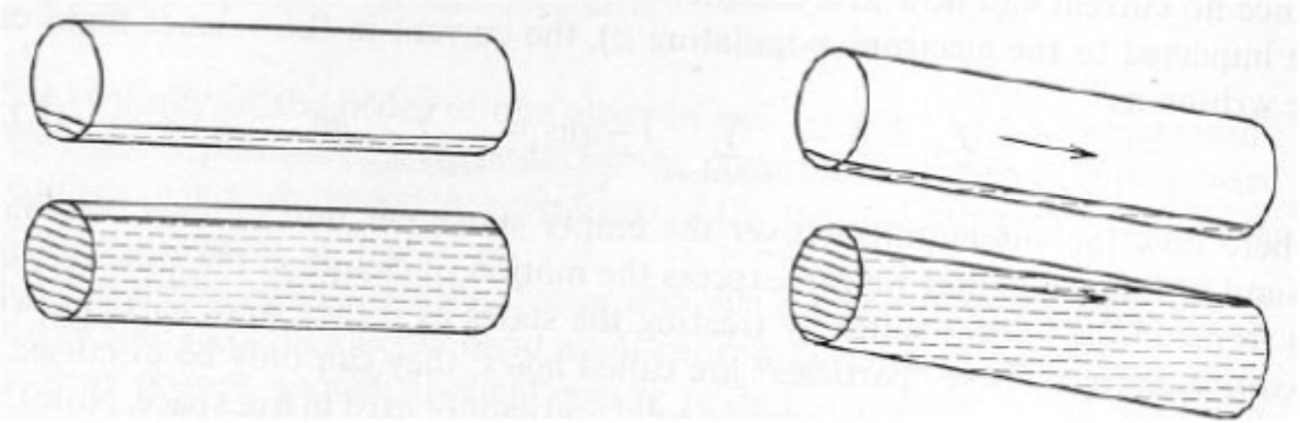


Some electrons receive enough thermal energy to be excited from valence band to conduction band

Hole

- What is a hole?
  - An empty state in the valence band
  - Treated as a positive charge carrier in the semiconductor

- Fluid analogy:



- Pure silicon at room temperature,
  - electron-hole pair density: 10^{10} EHP/cm^3
  - Silicon atom density: $5x10^{22}$ atom/cm^3
  - → electrons in the conduction band are free to move via many available empty states.

- Let's combine energy bands vs. k and vs. x:
- Note what is *potential*, *kinetic*, and *total* energy
- Note which way energy of *holes* increases

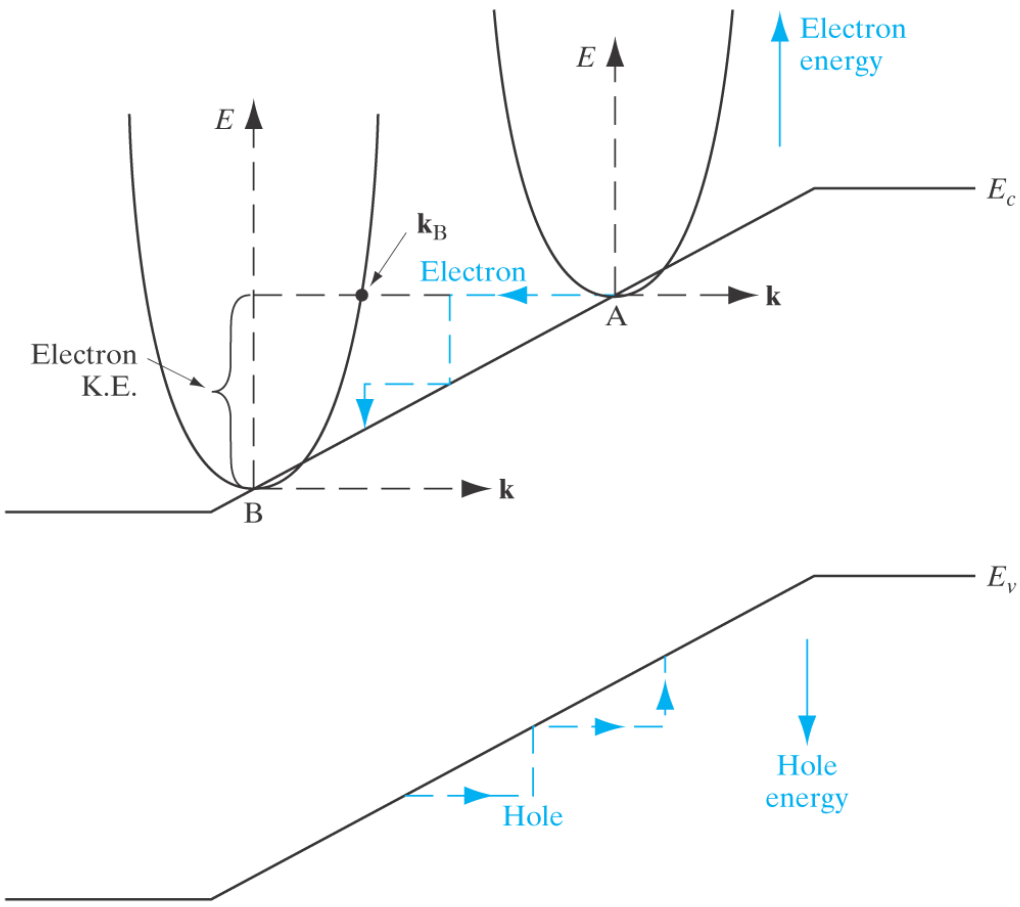
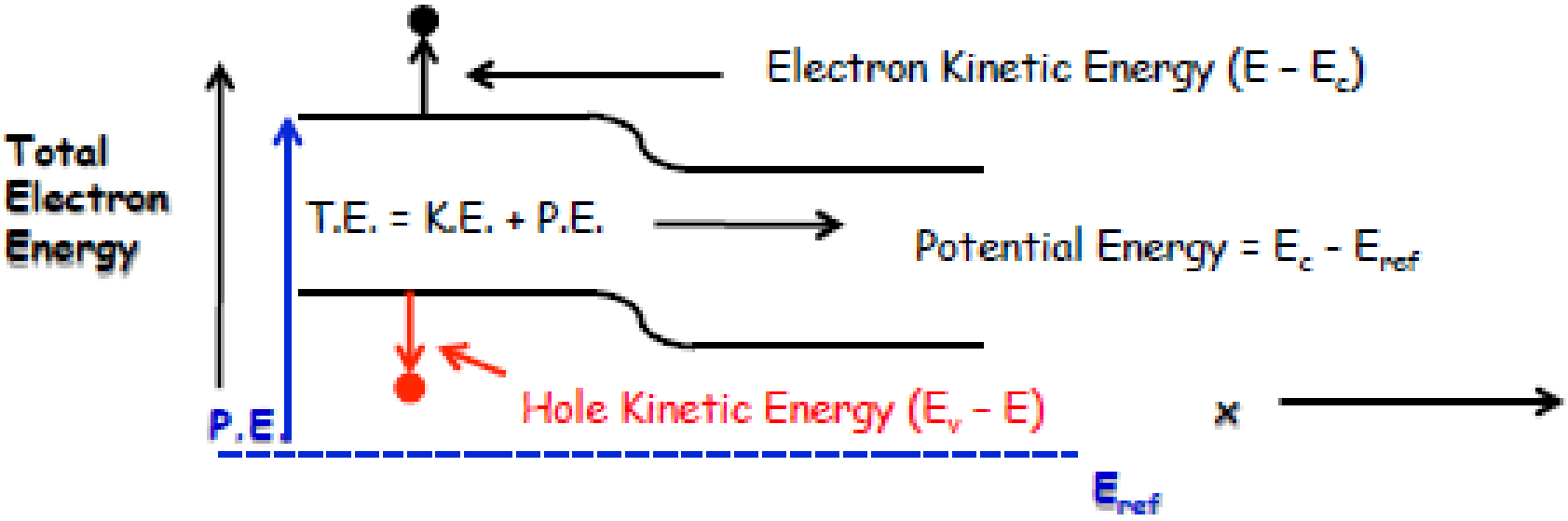


Figure 3.9

Superimposition of the (E,**k**) band structure on the E-versus-position simplified band diagram for a semiconductor in an electric field. Electron energies increase going up, while hole energies increase going down. Similarly, electron and hole wave vectors point in opposite directions and these charge carriers move opposite to each other, as shown.

Potential energy and kinetic energy



- **Hole energy increase oppositely to electron energy, because the two carriers have opposite charge**

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Effective Mass of electrons and holes

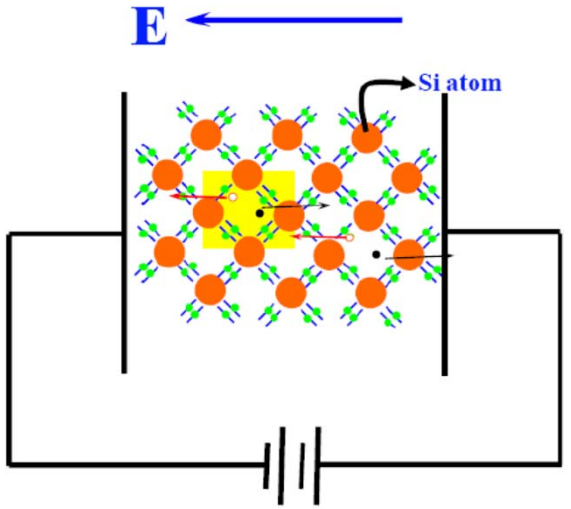
- Newton's law:

$$\boldsymbol{Force = F_{int} + F_{ext} = ma}$$

"true" mass, same as free electron mass $\boldsymbol{m_0}$

F_{int} is the collection of internal periodic crystal forces

$\boldsymbol{F_{ext}}$ is the externally applied force



- If the effect of all the internal periodic crystal forces are considered and encapsulated into the band structure. Then electron then respond to external force with a new mass:

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

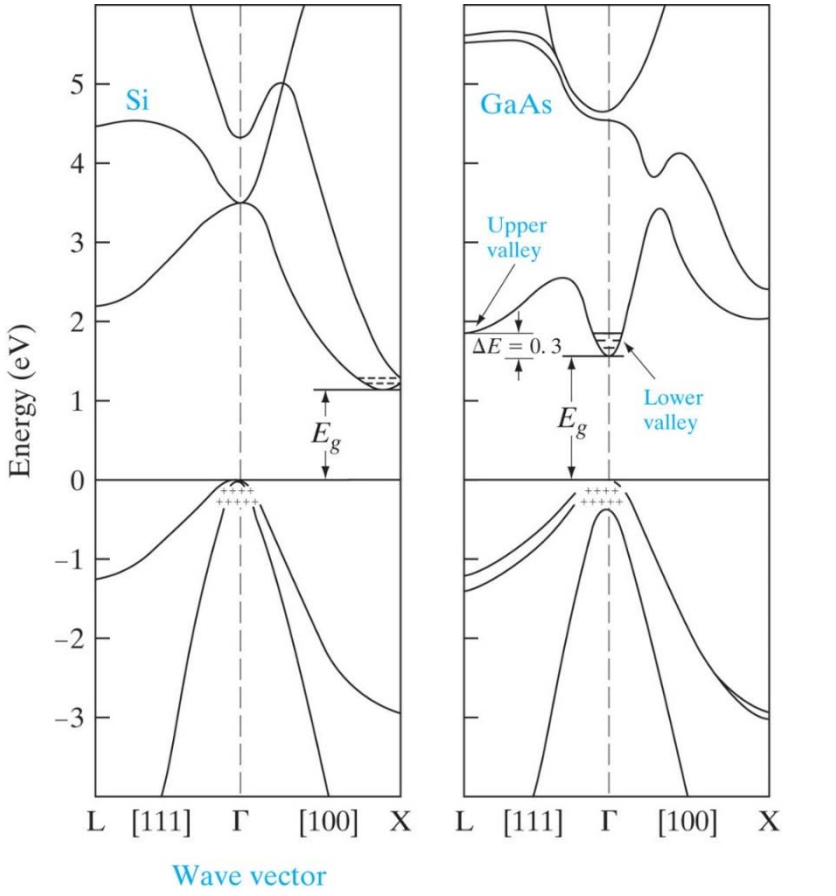
where m^* is the "effective mass" of the particle, which includes all the complex influences of the crystal potential on the motion of the electron (or hole).

Effective Mass

- The effective mass of a carrier in a solid is:

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

i.e, the curvature of the band determines the carrier effective mass

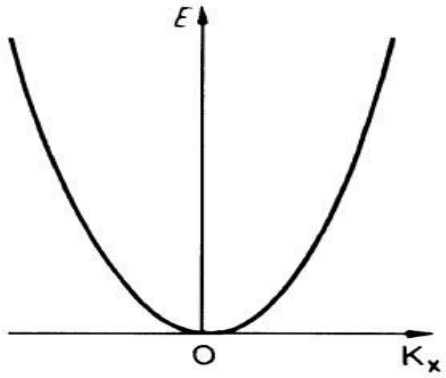


(a)

Effective Mass

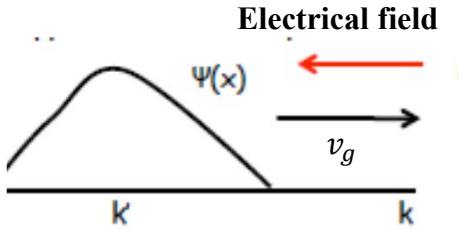
- Free electron energy is:

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



The electron mass is inversely related to the curvature of the (E,K) relationship:

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



- For electron in a solid, the group velocity of a quantum mechanical electron wavepacket is

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

The work done on the electron by the external force is: $\delta E = F_{ext} v_g \delta t \Rightarrow \frac{dk}{dt} = \frac{F_{ext}}{\hbar}$

$$\boldsymbol{m^* = \frac{F_{ext}}{dv_g/dt} = \frac{\hbar^2}{(d^2E)/(dk^2)}}$$

Effective Mass of electrons and holes

- Effective mass values? Fractions of m_0. See Appendix III.
  - Sometimes depend on direction of motion in the crystal.
  - E.g. for electrons in Si: $m_l = 0.98m_0$, $m_t = 0.19m_0$
  - Can also depend on particle location in the band (bottom, top, edge, “light” band vs. “heavy” band).
  - Values in Appendix III are given at the bottom of C-band for electrons, top of V-band for holes.

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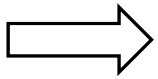
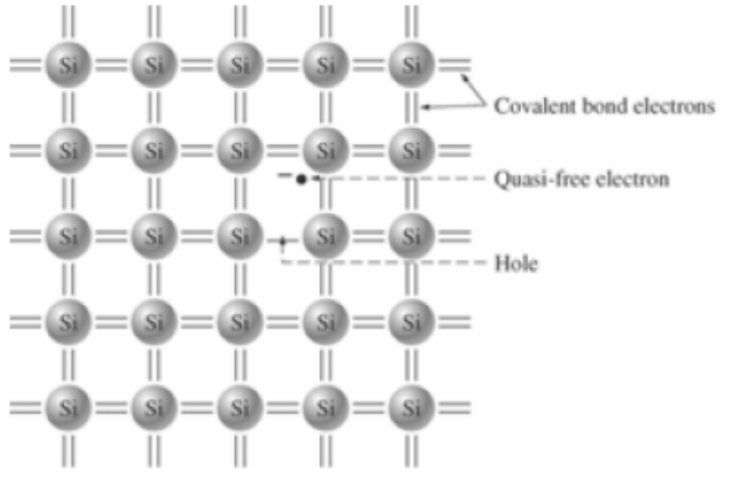
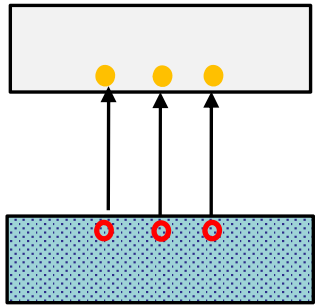
  - Intrinsic material
  - Extrinsic material



Intrinsic semiconductor

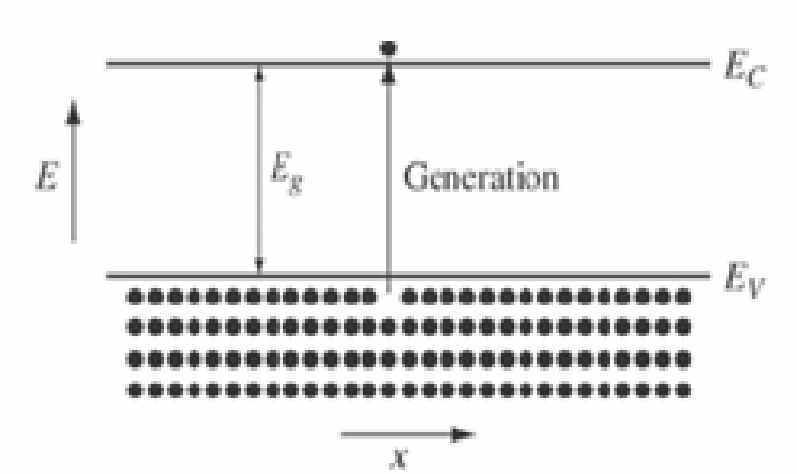
- Intrinsic semiconductor = pure, without external additives

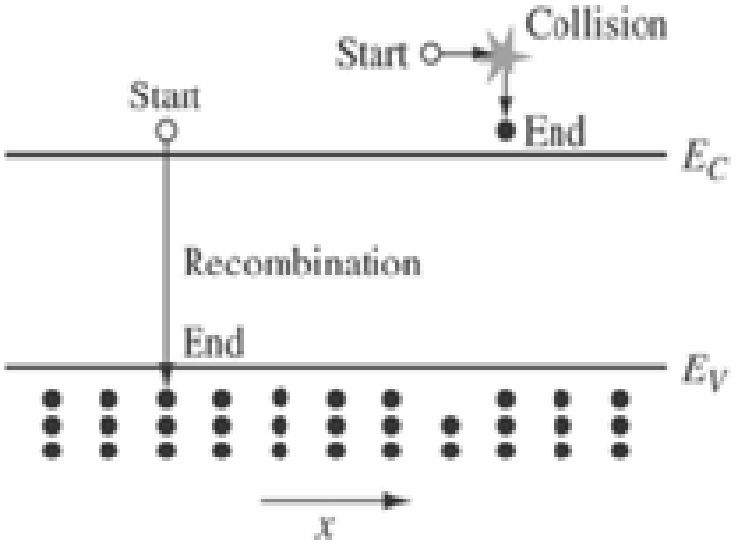




- No free charge carriers at T=0K
- What about at T=300K?
- How much energy to break a bond?

Generation and recombination in intrinsic semiconductor

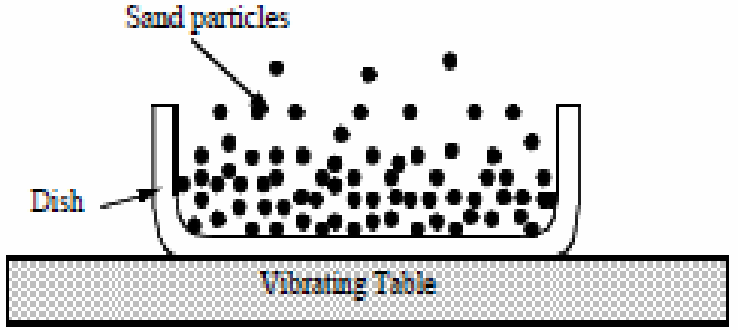




Electron and home generate in pairs and recombine in pairs.

$$\boldsymbol{n = p = n_i}$$

n: electron concentration
p: hole concentration
n_i: intrinsic carrier concentration



Mechanical analogy:

Generation and recombination rate

- Generation rate of EHP g_i is determined by the temperature and bandgap:
  - High T → _higher or lower?_ generation rate
  - Small band gap → _higher or lower?_ generation rate
- Recombination rate is determined by the number of electron and hole concentration:

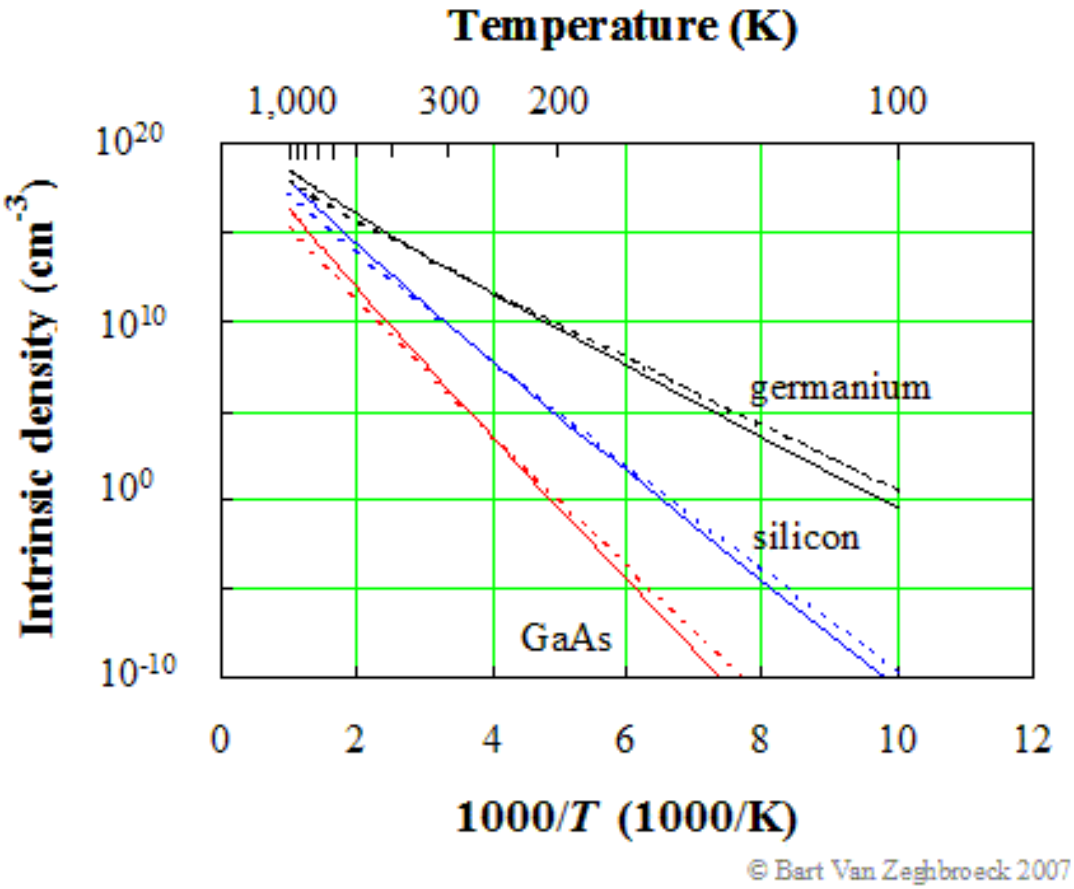
$$r_i = \alpha n_0 p_0 = \alpha n_i^2$$

- At equilibrium:

$$r_i = g_i = \alpha n_i^2$$

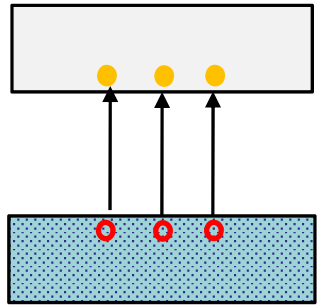
Question: How is the intrinsic carrier concentration change with temperature and band gap?

Intrinsic carrier concentration as a function of temperature



How does n_i change with T?
Which curve is for GaAs, Si, Ge?

GaAs: $E_G \approx 1.42$ eV
Si: $E_G \approx 1.12$ eV
Ge: $E_G \approx 0.67$ eV

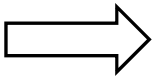


Intrinsic carrier density versus temperature in gallium arsenide (GaAs), silicon and germanium. Compared is the calculated density with (solid lines) and without (dotted lines) the temperature dependence of the energy bandgap

For Silicon at room temperature, intrinsic carrier density $n_i \cong 10^{10}\ cm^{-3}$

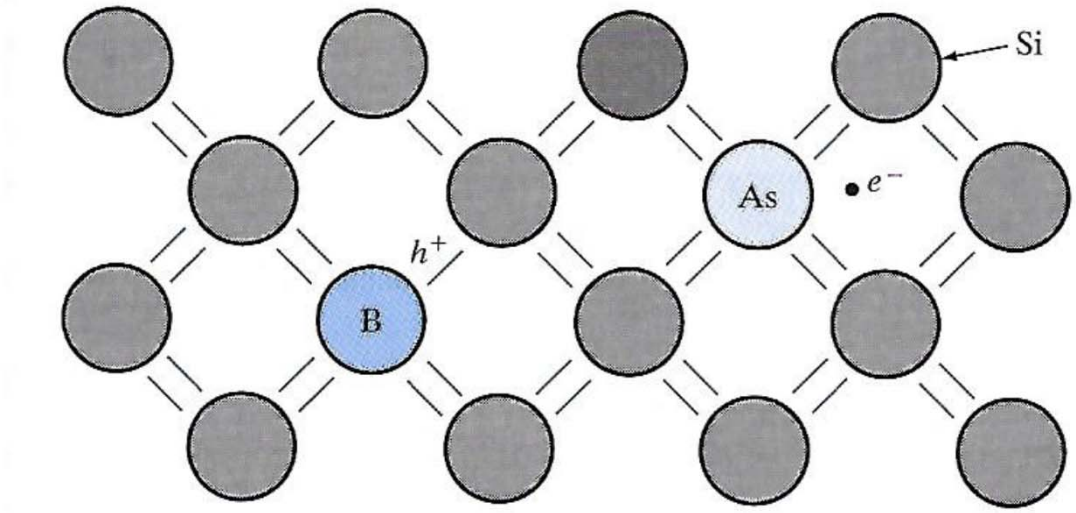
Outline

- Bonding force and energy band
  - Bonding forces in solids
  - Energy bands
  - Metals, semiconductors, and insulators
  - Direct and indirect semiconductors
- Charge carriers in semiconductors
  - Electrons and holes
  - Effective mass
  - Intrinsic material
  - Extrinsic material



Extrinsic material

- How to manipulating the carrier concentration?
- Doping = purposely introducing impurities into the crystal
- *Intrinsic* material = pure, undoped. *Extrinsic* = doped.

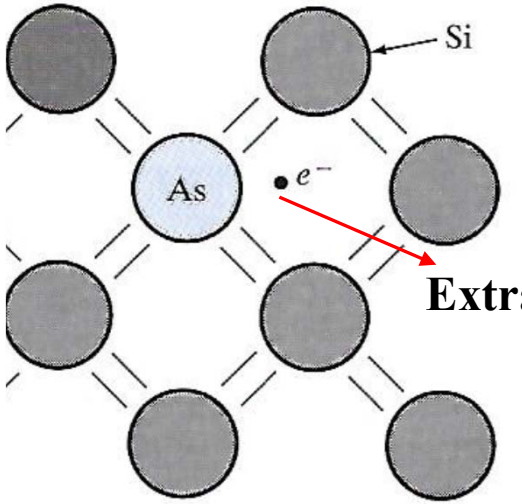


	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

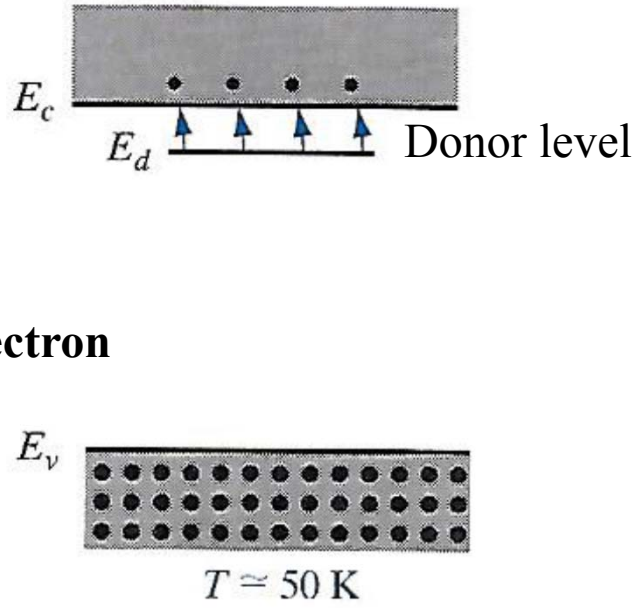
N type doping

Example: Add column V elements (P, As etc) into Si or Ge crystal:

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	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



Extra electron



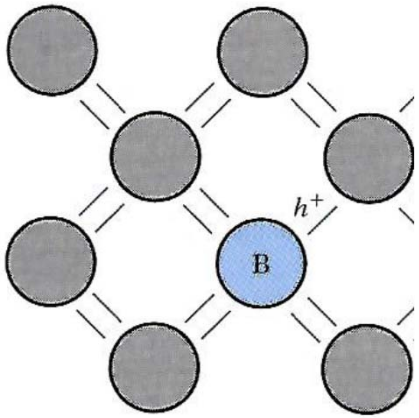
- Electron concentration is much higher than holes

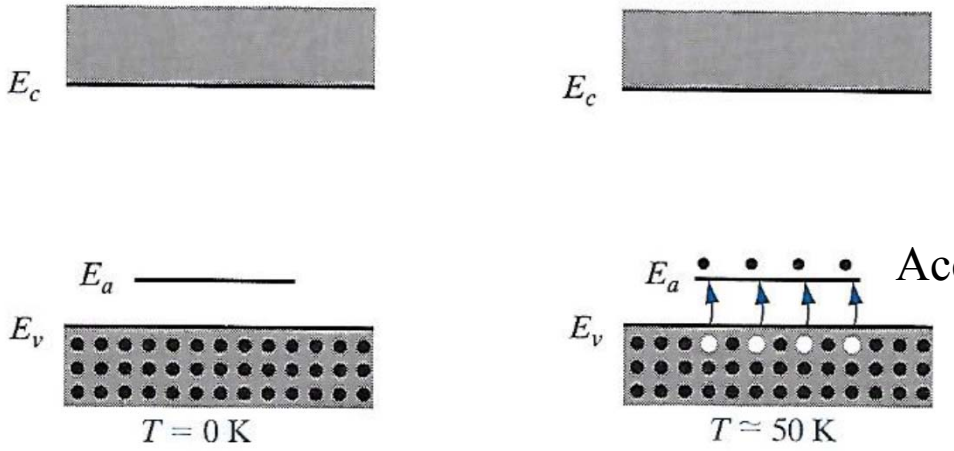
$$n_0 \gg p_0 \; or \; n_i$$

called **n type** material.

P type doping

Example: adding column III element to Si or Ge crystal:





Acceptor level

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	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

- The impurity introduce an energy level very near the **valence band**. This type of impurity level "accept" electron from valence band and are called "**acceptor**" impurity.
- Hole concentration is much higher than electrons

$$p \gg n_0 \; or \; n_i$$

called **p type** material.

Binding energy

- Arsenic (As) dopant in Si: 4 electrons used up for bonding with neighbors. But, how loosely bound is that 5th electron that As brought into the Si lattice?
- Approximate binding energy using Niels Bohr's model:

$$E_B \approx \frac{m^* q^4}{2K^2\hbar^2}$$

be careful with choice of m^* and $K = 4\pi\epsilon_r\epsilon_0$

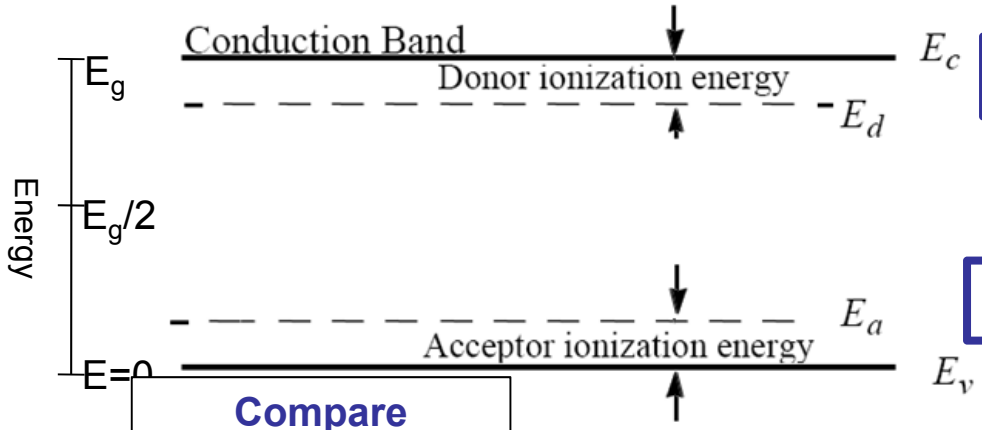
- The real numbers of donors and acceptors in Si:

Donor in Si	P	As	Sb
Binding energy (eV)	0.045	0.054	0.039

Acceptor in Si	B	Al	Ga	In
Binding energy (eV)	0.045	0.067	0.072	0.16

- (note: binding energy = ionization energy)

Typical Impurity Ionization Energy in Silicon

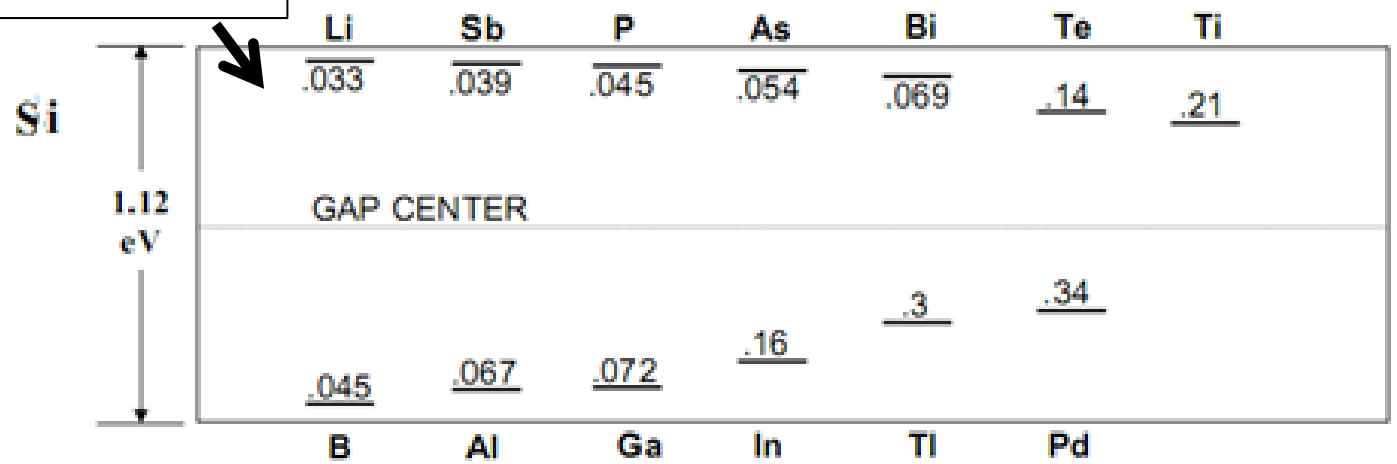


Donor Ionization Energy: $E_{I,donor} = E_C - E_d$

Acceptor Ionization Energy: $E_{I,acceptor} = E_a - E_V$

Compare to thermal energy kT=0.0259eV

Typical Ionization Energy in Silicon



Question

- If use Si to replace Ga in GaAs? Is Si atom server as donor or acceptor?

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	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

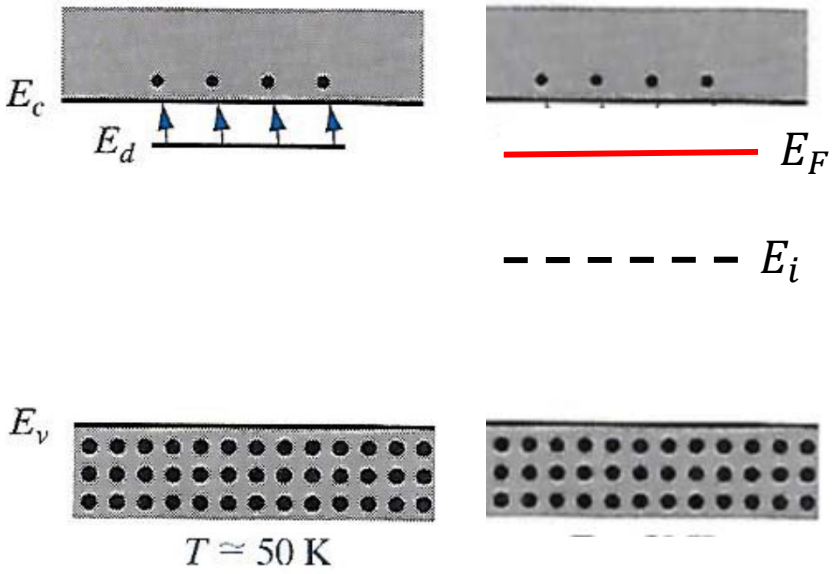
N type Doping

- If the impurity atoms has more valence electrons than original atoms in the lattice:

Use column	to replace
VI	V
V	IV
IV	III
III	II

extra electron will be donated

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	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



➔ N type doping

$$n_0 > p_0$$

$$E_F > E_i$$

P type Doping

- If the impurity atoms has less valence electrons than original atoms in the lattice:

Use column	to replace
V	VI
IV	V
III	IV
II	III

  - missing electron will create "holes"

➔ P type doping

$$p_0 > n_0$$

$$E_F < E_i$$

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	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