

*EE415/515 Fundamentals
of Semiconductor Devices
Fall 2012*

**Lecture 2: Energy bands
(Chapter 3.1-3.3)**

Today's Questions

- What are the different types of solids?
- How are the atoms arranged in a solid?
- What influences the arrangement?
- Why are the states in a solid different from those in isolated atoms or molecules?
- How does that arrangement influence the electrical characteristics of the material?
- What is a semiconductor?
- How do we develop the band model from all this?

Overview

- Structure of solids and how different properties arise.
 - Metal
 - Insulator
 - Semiconductor
- Energy bands and forbidden gaps
- Effective mass

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How to Model Solids

- Bond model: Consider bonds between many individual atoms.
 - Great visual model, important for intuition.
- Energy band model: Consider energy bands of individual atoms and how they combine and deform when brought together.
 - Good for understanding energy related topics like energy gaps.

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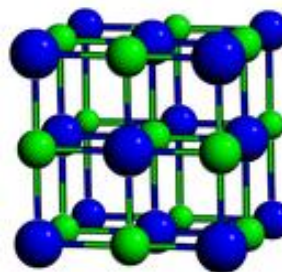
Bond Model of Solids

- Ionic: electrons shifted to one atom to complete shell. Very strong.
- Metallic: partially filled outer shells lead to essentially “free” “sea of electrons.”
- Covalent: electrons shared fairly equally. Quantum interactions lead to bonding.

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Ionic Bonding in Solids

- Ionic bonding (NaCl). Each Na atom surrounded by six Cl and vice versa.
- Na is $[\text{Ne}]3s^1$ and Cl is $[\text{Ne}]3s^23p^5$
- In the lattice each Na gives up the electron to a Cl.
- Ions have electronic structure of inert atoms, but are charged and therefore attract.
- Electrons are tightly bound.
- Therefore NaCl is a good insulator.



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Metallic Bonding

- Outer shell only partially filled.
 - E.g. alkali metals have only one electron which is easily given up.
 - Good chemical activity and electrical conductivity.
- Solid made of ions with closed shells and free electrons.
 - Interaction forces cause metallic bonding.

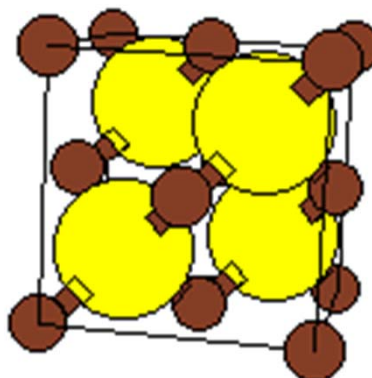
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III-V compounds

- Zincblende lattice: In some compound semiconductors atoms in the diamond structure differ on alternating sites.
- Can vary the mixture of elements which allows control of electronic and optical properties of the material.

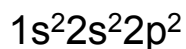
[GaAs Unit Cell applet](http://jas.eng.buffalo.edu/education/solid/unitCell/home.html)

(<http://jas.eng.buffalo.edu/education/solid/unitCell/home.html>)



How are elements like carbon configured at the atomic level?

- First check periodic chart. Atomic number = 6.
- Find out how many valence electrons.
- Then figure out the electronic configuration:



- But when it comes to *bonding in a solid* it will be energetically favorable to have equal bonds between equal orbitals.

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Hybridization

- Sometimes the outer orbitals will combine in a manner called hybridization.
- In elements like carbon and silicon it is a lower energy orbital combination.
- So you actually get four equal sp^3 hybrids which are tetragonal, rather than s^2p^2 .



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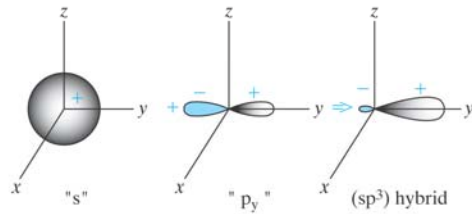


Figure 2.9

Orbitals in a Si atom: The spherically symmetric "s" type wave functions or orbitals are positive everywhere, while the three mutually perpendicular "p" type orbitals (p_x , p_y , p_z) are dumbbell shaped and have a positive lobe and a negative lobe. The four sp^3 "hybridized" orbitals, only one of which is shown here, point symmetrically in space and lead to the diamond lattice in Si.

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2D representations

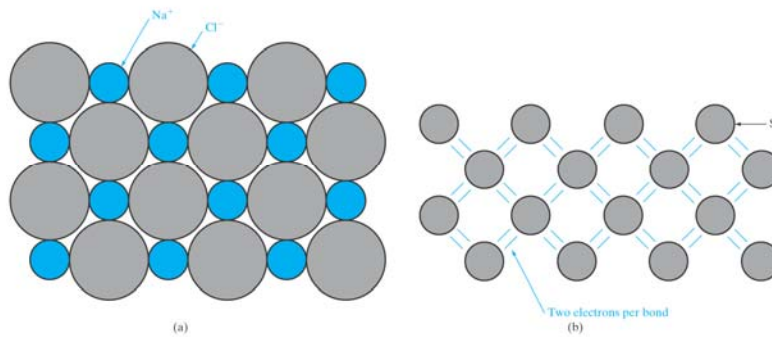


Figure 3.1

Different types of chemical bonding in solids: (a) an example of ionic bonding in NaCl; (b) covalent bonding in the Si crystal, viewed along a $\langle 100 \rangle$ direction (see also Figs. 1-8 and 1-9).

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Covalent Solids

- Silicon and germanium have a diamond-type crystal lattice. Each atom has covalent bonds with four neighbors.
- Two tightly bound electrons for each bond.
- At absolute zero all electrons are tightly bound.
- At higher temperatures bonds break creating nearly free electrons and empty bonds.
- Empty bond appears like a positive charge.

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Energy bands in solids

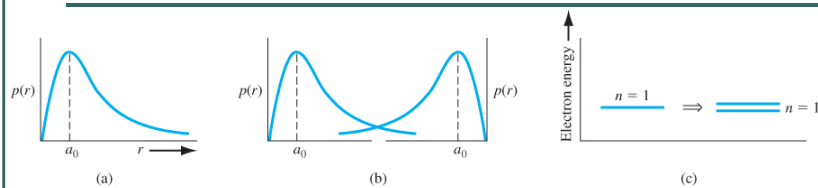


Figure 3.1 | (a) Probability density function of an isolated hydrogen atom. (b) Overlapping probability density functions of two adjacent hydrogen atoms. (c) The splitting of the $n = 1$ state.

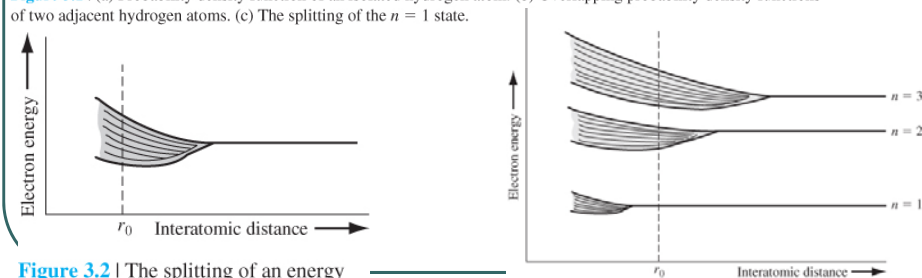
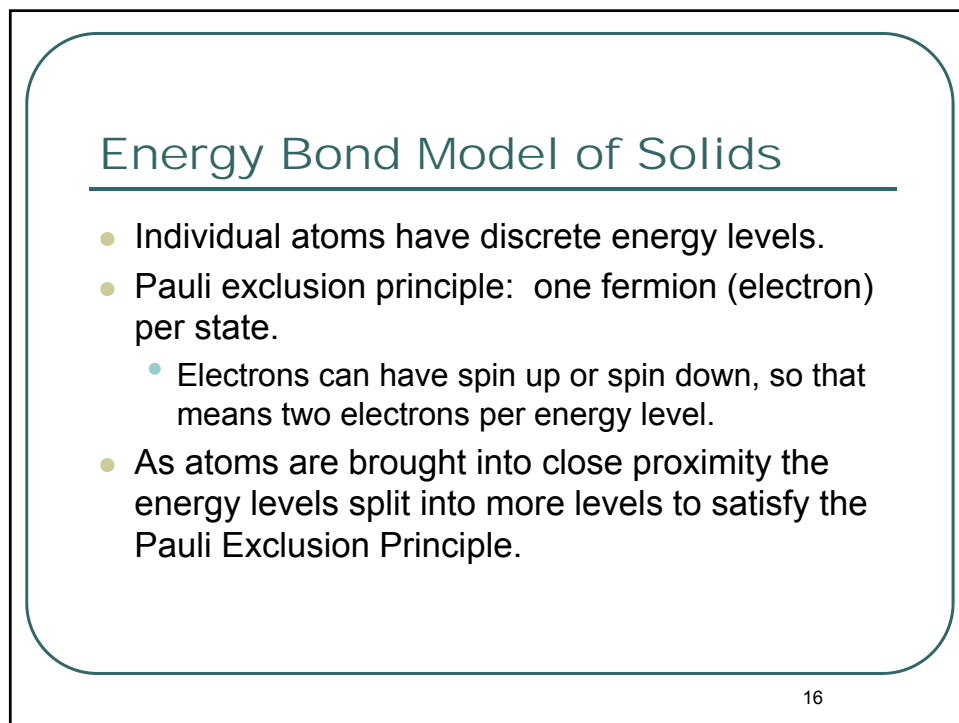
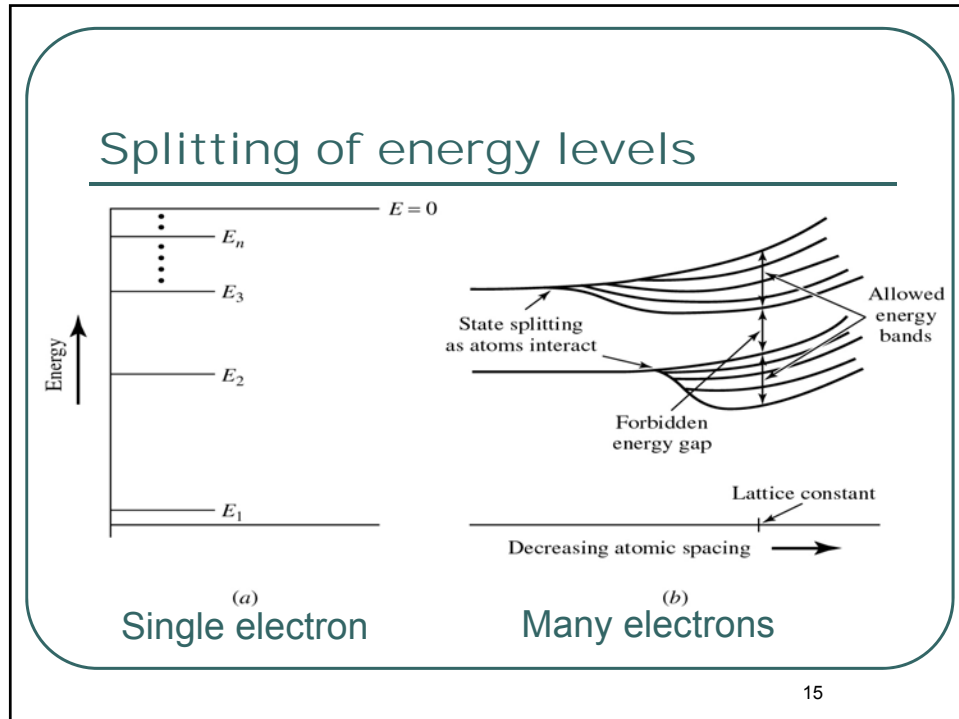


Figure 3.2 | The splitting of an energy state into a band of allowed energies.

Figure 3.3 | Schematic showing the splitting of three energy states into allowed bands of energies.



Two atoms \rightarrow energy levels split into two

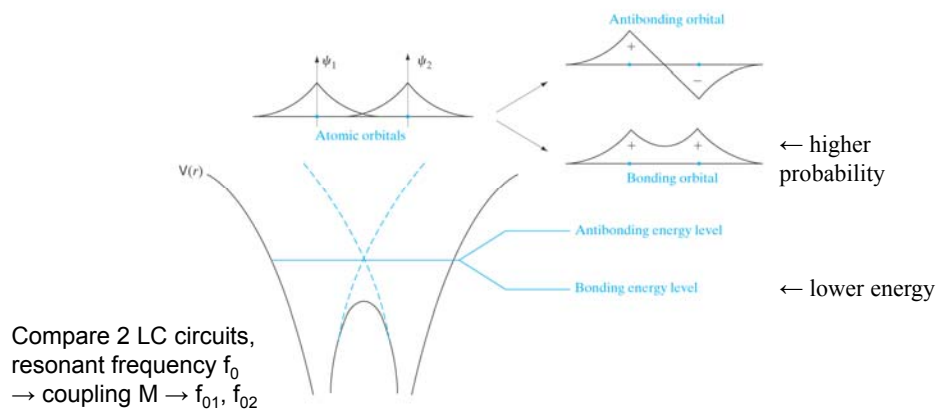


Figure 3.2

Linear combinations of atomic orbitals (LCAO): The LCAO when 2 atoms are brought together leads to 2 distinct "normal" modes—a higher energy antibonding orbital, and a lower energy bonding orbital. Note that the electron probability density is high in the region between the ion cores (covalent "bond"), leading to lowering of the bonding energy level and the cohesion of the crystal. If instead of 2 atoms, one brings together N atoms, there will be N distinct LCAO, and N closely spaced energy levels in a band.

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Energy Bands

- Two electron wave functions are linear combinations of the individual atomic orbitals (LCAO.)
 - Odd is called anti-bonding, which is a higher energy level.
 - Even is called bonding, which is a lower energy level.
 - Lower energy holds crystal together.
- As many atoms are brought together the split levels form continuous bands of energies.
 - Note that this is a *mental* model for visualization.

Energy levels split into bands

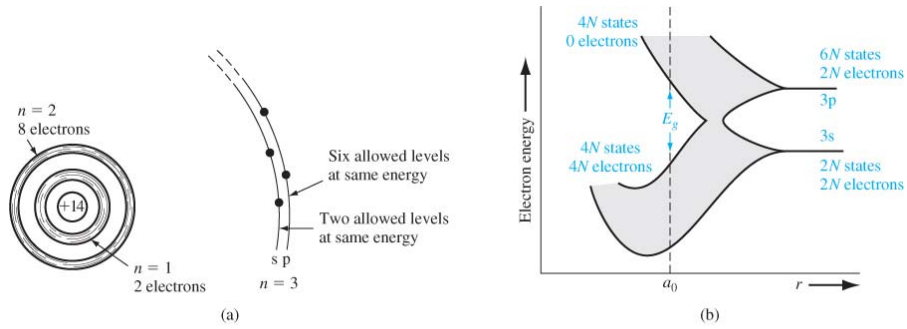


Figure 3.4 | (a) Schematic of an isolated silicon atom. (b) The splitting of the 3s and 3p states of silicon into the allowed and forbidden energy bands.
(From Shockley [6].)

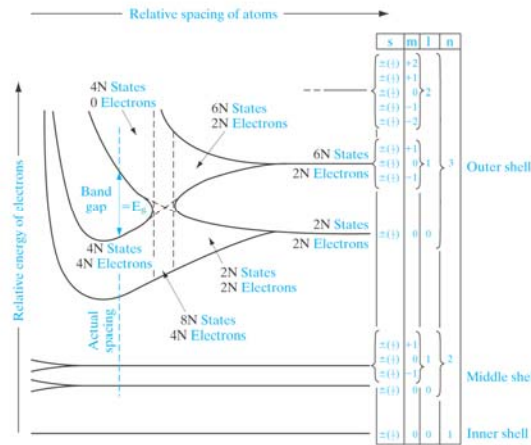


Figure 3.3

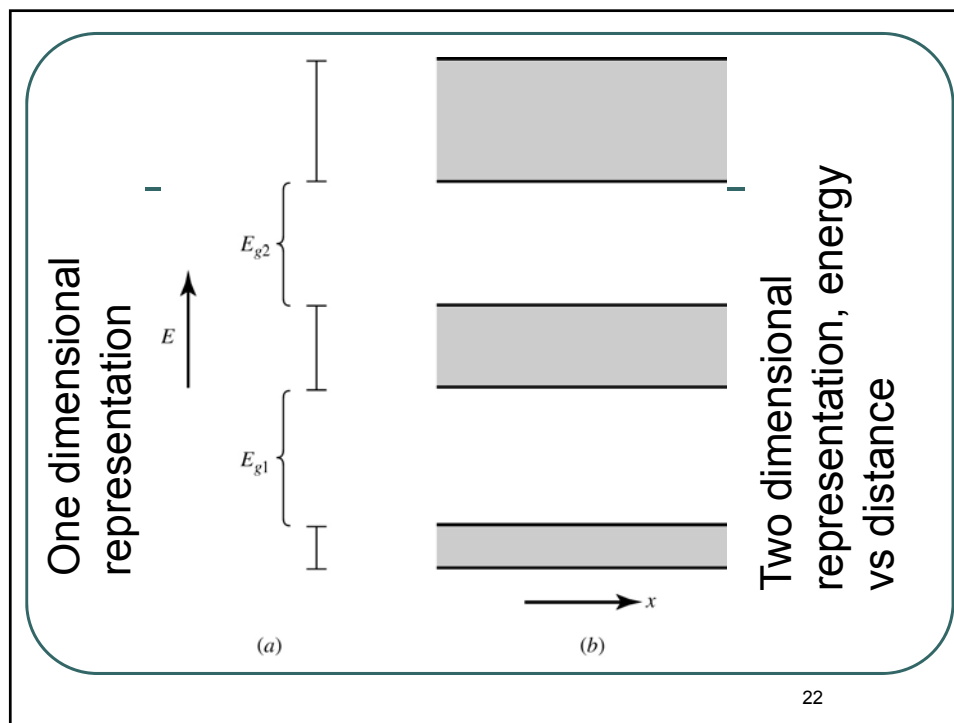
Energy levels in Si as a function of interatomic spacing. The core levels ($n = 1, 2$) in Si are completely filled with electrons. At the actual atomic spacing of the crystal, the $2N$ electrons in the $3s$ subshell and the $2N$ electrons in the $3p$ subshell undergo sp^3 hybridization, and all end up in the lower $4N$ states (valence band), while the higher-lying $4N$ states (conduction band) are empty, separated by a band gap.

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Energy bands in Silicon

- N atoms brought into crystal lattice.
 - 2N electrons from the 3s states.
 - 2N electrons from the 6p states.
 - 4N electrons available for 8N states.
- As the spacing decreases the energy states split into bands separated by an energy gap E_g .
 - Upper “conduction” band contains 4N states.
 - Lower “valence” band contains 4N states.
 - At 0K every state in valence band will be filled.

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Kronig-Penney Model

Model is a demonstration of the band structure of solids and of effective electron mass.

No quantitative results.

Periodic potential of a 1D crystal lattice →

Figure 3.5 | (a) Potential function of a single isolated atom. (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.

Kronig-Penney Model (energy bands and effective mass)

Note: Rectangular potential approximation
Shift in $V(x)$ zero reference
 $u(x)$ periodic in $(a+b)$

Figure 3.6 | The one-dimensional periodic potential function of the Kronig-Penney model.

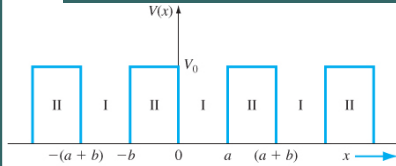
Wavefunction $\Psi(x,t) = \psi(x)\phi(t) = u(x)e^{jkx}e^{-j(E/\hbar)t} = u(x)e^{j(kx - (E/\hbar)t)}$

where $\psi(x) = u(x)e^{jkx}$, so $\frac{d\psi}{dx} = jku(x)e^{jkx} + e^{jkx} \frac{du}{dx}$

and $\frac{d^2\psi(x)}{dx^2} = -k^2u(x)e^{jkx} + jke^{jkx} \frac{du(x)}{dx} + jke^{jkx} \frac{du(x)}{dx} + e^{jkx} \frac{d^2u(x)}{dx^2}$

$$= e^{jkx} \left[\frac{d^2u(x)}{dx^2} + 2jk \frac{du(x)}{dx} - k^2u(x) \right]$$

Kronig-Penney Model (energy bands and effective mass)



So $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$ gives :

$$\frac{d^2u(x)}{dx^2} + 2jk \frac{du(x)}{dx} - (k^2 - \alpha^2)u(x) - \frac{2m}{\hbar^2}V(x)u(x) = 0$$

where $\alpha^2 = \frac{2mE}{\hbar^2}$

Figure 3.6 | The one-dimensional periodic potential function of the Kronig-Penney model.

In Region I, $V(x) = 0$ & $\frac{d^2u_1(x)}{dx^2} + 2jk \frac{du_1(x)}{dx} - (k^2 - \alpha^2)u_1(x) = 0$

with solution $u_1(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha-k)x}$ for $0 < x < a$

In Region II, $V(x) = V_0$ & $\frac{d^2u_2(x)}{dx^2} + 2jk \frac{du_2(x)}{dx} - (k^2 - \beta^2)u_2(x) = 0$

where $\beta^2 = \alpha^2 - \frac{2m}{\hbar^2}V_0 = \frac{2m}{\hbar^2}(E - V_0)$

with solution $u_2(x) = Ce^{j(\beta-k)x} + De^{-j(\beta-k)x}$ for $-b < x < 0$

Kronig-Penney Model (energy bands and effective mass)

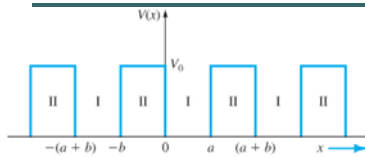


Figure 3.6 | The one-dimensional periodic potential function of the Kronig-Penney model.

Boundary conditions :

$x = 0 \quad u_1(0) = u_2(0) \rightarrow A + B = C + D$

$$\left. \frac{du_1}{dx} \right|_{x=0} = \left. \frac{du_2}{dx} \right|_{x=0} \rightarrow (\alpha - k)A - (\alpha + k)B = (\beta - k)C - (\beta + k)D$$

Periodicity:

$u_1(a) = u_2(b) \rightarrow Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} = Ce^{-j(\beta-k)b} + De^{j(\beta+k)b}$

$$\left. \frac{du_1}{dx} \right|_{x=a} = \left. \frac{du_2}{dx} \right|_{x=b} \rightarrow (\alpha - k)Ae^{j(\alpha-k)a} - (\alpha + k)Be^{-j(\alpha+k)a} = (\beta - k)Ce^{-j(\beta-k)b} - (\beta + k)De^{j(\beta+k)b}$$

Kronig-Penney Model (energy bands and effective mass)

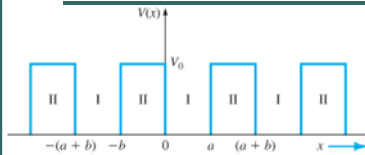


Figure 3.6 | The one-dimensional periodic potential function of the Kronig-Penney model.

Solve 4 equations to get :

$$\frac{-(\alpha^2 + \beta^2)}{2\alpha\beta} (\sin \alpha a)(\sin \beta b) + (\cos \alpha a)(\cos \beta b) = \cos k(a+b)$$

For electrons in the crystal, $E < V_0$, so $\beta = \sqrt{2m(E-V_0)}/\hbar = j\gamma$, and

$$\frac{(\gamma^2 - \alpha^2)}{2\alpha\gamma} (\sin \alpha a)(\sinh \gamma b) + (\cos \alpha a)(\cosh \gamma b) = \cos k(a+b)$$

Simplify with $b \rightarrow 0, V_0 \rightarrow \infty$, with bV_0 finite, gives

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad \text{where} \quad P = \frac{mV_0 b a}{\hbar^2}$$

Kronig-Penney Model (energy bands and effective mass)

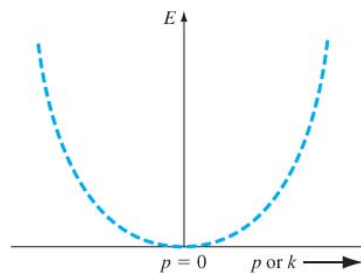


Figure 3.7 | The parabolic E versus k curve for the free electron.

Special Case : $V_0 = 0$ (free electron) $\rightarrow P = 0$
then $\cos \alpha a = \cos ka \rightarrow \alpha = k$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m\left(\frac{1}{2}mv^2\right)}{\hbar^2}} = \frac{p}{\hbar} = k$$

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

$$E = \frac{\hbar^2}{2m} k^2 \quad \text{for free electron}$$

Kronig-Penney Model (energy bands and effective mass)

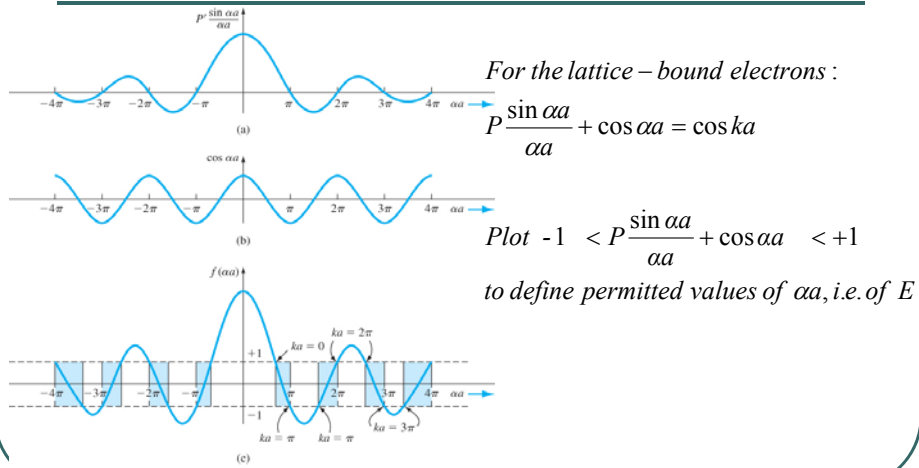


Figure 3.8 | A plot of (a) the first term in Equation (3.29), (b) the second term in Equation (3.29), and (c) the entire $f(\alpha a)$ function. The shaded areas show the allowed values of αa corresponding to real values of k .

Kronig-Penney Model (energy bands and effective mass)

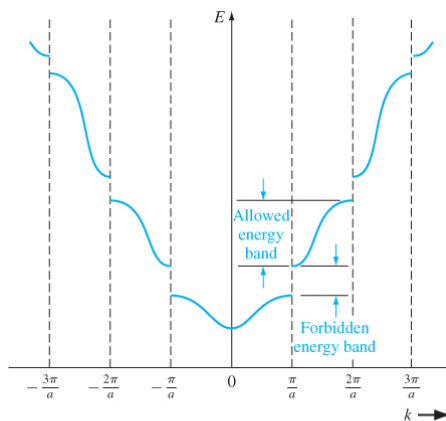


Figure 3.9 | The E versus k diagram generated from Figure 3.8. The allowed energy bands and forbidden energy bandgaps are indicated.

Kronig-Penney Model

$\cos(ka) = \cos(ka+2n\pi) = \cos(ka-2n\pi)$, so can collapse figure

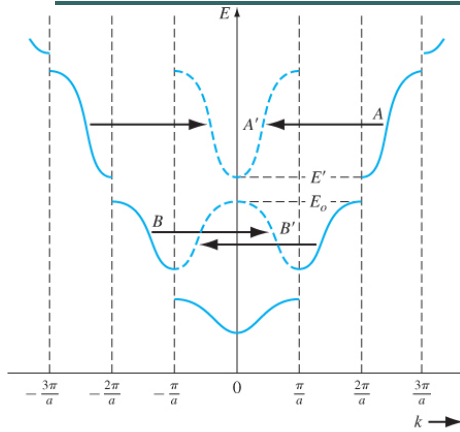


Figure 3.10 | The E versus k diagram showing 2π displacements of several sections of allowed energy bands.

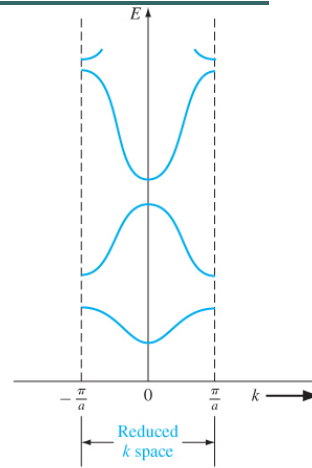


Figure 3.11 | The E versus k diagram in the reduced-zone representation.

Electron conduction: electron-hole pairs (EHPs)

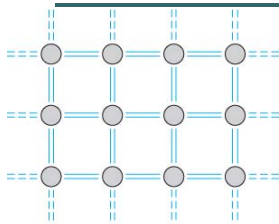


Figure 3.12 | Two-dimensional representation of the covalent bonding in a semiconductor at $T = 0$ K.

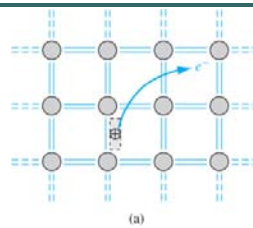


Figure 3.13 | (a) Two-dimensional representation of the breaking of a covalent bond. (b) Corresponding line representation of the energy band and the generation of a negative and positive charge with the breaking of a covalent bond

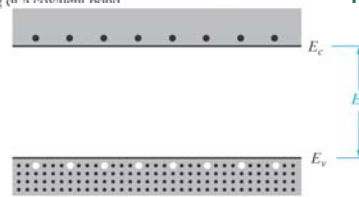
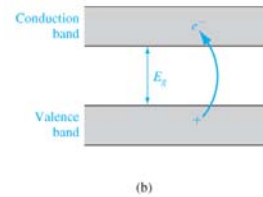


Figure 3.7

Electron-hole pairs in a semiconductor.

Intrinsic: Electron-hole pairs (EHPs)

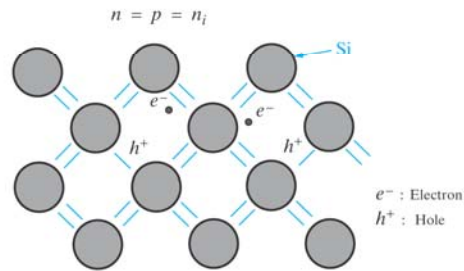


Figure 3.11

Electron-hole pairs in the covalent bonding model of the Si crystal.

$$n_0 = p_0 = n_i \therefore n_0 p_0 = n_i^2$$

$$\text{At equilibrium } r_i = g_i = \alpha_r n_0 p_0 = \alpha_r n_i^2$$

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Electron conduction: drift current

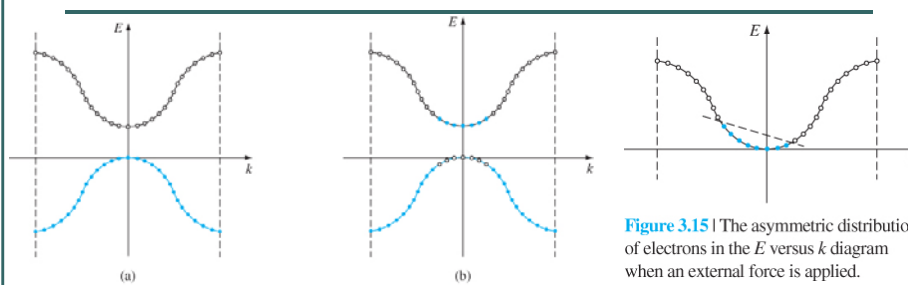


Figure 3.14 | The E versus k diagram of the conduction and valence bands of a semiconductor at (a) $T = 0$ K and (b) $T > 0$ K.

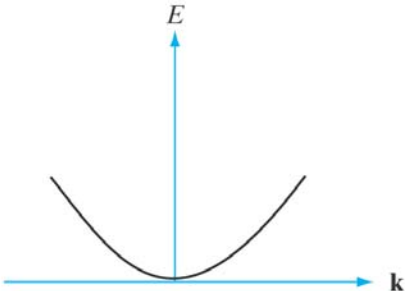
Figure 3.15 | The asymmetric distribution of electrons in the E versus k diagram when an external force is applied.

Drift current :

$$J = q \sum_{i=1}^N v_i = q N v_d \text{ A/cm}^2 \text{ where } v_d = \text{average drift velocity}$$

Note shift in $E - k$ distribution due to net momentum in applied field.

Effective Mass



E

k

Momentum $p = \hbar k = \frac{\hbar}{2\pi} k$

Energy $E = \frac{1}{2} m v^2 = \frac{p^2}{2m} = \frac{\hbar^2}{2m} k^2$

$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar p}{m}$, i.e. $v = \frac{p}{m} = \frac{1}{\hbar} \frac{dE}{dk}$

and $\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$, or $m = \frac{\hbar^2}{d^2 E/dk^2}$

and if E vs k is ~ parabolic at the bottom of the conduction band,

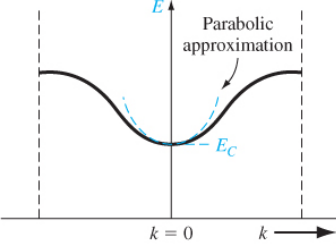
then $E - E_c = C_1 k^2$, so $\frac{d^2 E}{dk^2} = 2C_1$ and $m^* = \frac{\hbar^2}{2C_1}$

where m^* is the effective mass

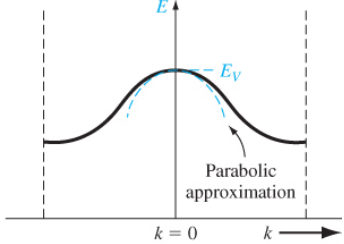
Note : Effective mass constant at the bottom of the conduction band, or where E vs k is parabolic (free electron)

Electron acceleration $a = \frac{(-e)E}{m_n^*}$

Parabolic band approximation and hole concept



(a)



(b)

Figure 3.16 (a) The conduction band in reduced k space, and the parabolic approximation. (b) The valence band in reduced k space, and the parabolic approximation.

In valence band : $E - E_v = -C_2 k^2$ gives $m^* = \frac{\hbar^2}{d^2 E/dk^2} = -\frac{\hbar^2}{2C_2}$

i.e. electron at the top of the valence band has negative effective mass

Consider current carried by holes of charge $+e$ and positive effective mass m_p^*

Completely filled valence band:

$$J = -q \sum_1^N v_i = 0$$

Remove electron \rightarrow hole

$$J = -q \sum_1^N v_i - (-q)v_j = qv_j$$

(positive charge)

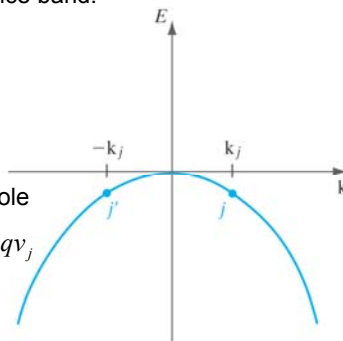


Figure 3.8

A valence band with all states filled, including states j and j' , marked for discussion. The j th electron with wave vector k_j is matched by an electron at j' with the opposite wave vector $-k_j$. There is no net current in the band unless an electron is removed. For example, if the j th electron is removed, the motion of the electron at j' is no longer compensated.

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Charge transport

- For electrons in solids to move there must be available empty states.
- In Si at 0K the valence band is completely filled and the conduction band is completely empty.
 - No charge transport.
- Insulators are the same, however the band gap is larger in an insulator than in silicon.
 - Silicon $E_b = 1.1\text{eV}$. Small enough to allow excitation into the conduction band from thermal or optical energy.
 - Diamond $E_g = 5\text{eV}$
- Metals have overlapping or partially filled bands.
 - Many charges available to move (conduction).

Hole conduction

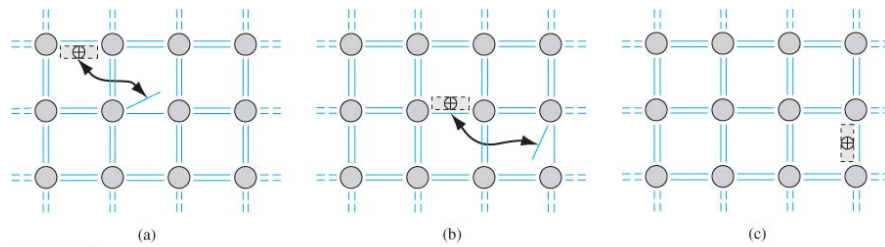


Figure 3.17 | Visualization of the movement of a hole in a semiconductor.

Lecture 1b p.39
Introduction

Hole conduction

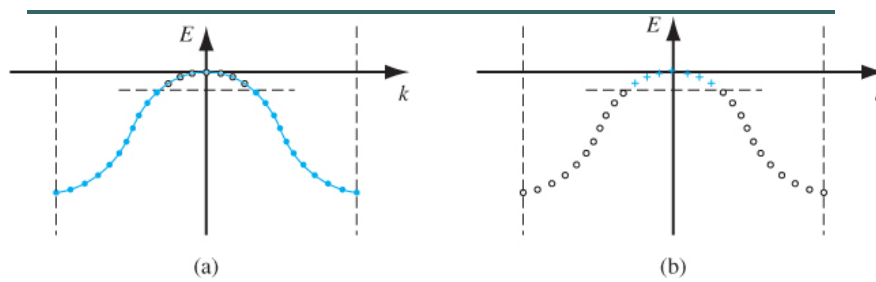


Figure 3.18 | (a) Valence band with conventional electron-filled states and empty states. (b) Concept of positive charges occupying the original empty states.

Lecture 1b p.40
Introduction

Semiconductors: $T=0K$ & $T>0K$

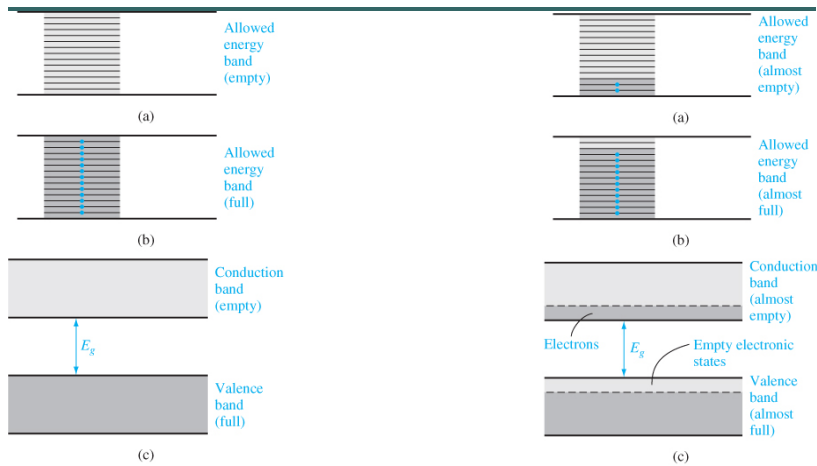


Figure 3.19 | Allowed energy bands showing (a) an empty band, (b) a completely full band, and (c) the bandgap energy between the two allowed bands.

Figure 3.20 | Allowed energy bands showing (a) an almost empty band, (b) an almost full band, and (c) the bandgap energy between the two allowed bands.

Metals

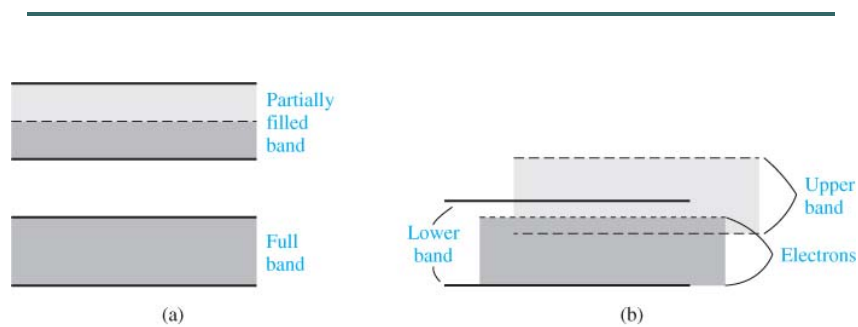


Figure 3.21 | Two possible energy bands of a metal showing (a) a partially filled band and (b) overlapping allowed energy bands.

Insulator, semiconductor, & metal

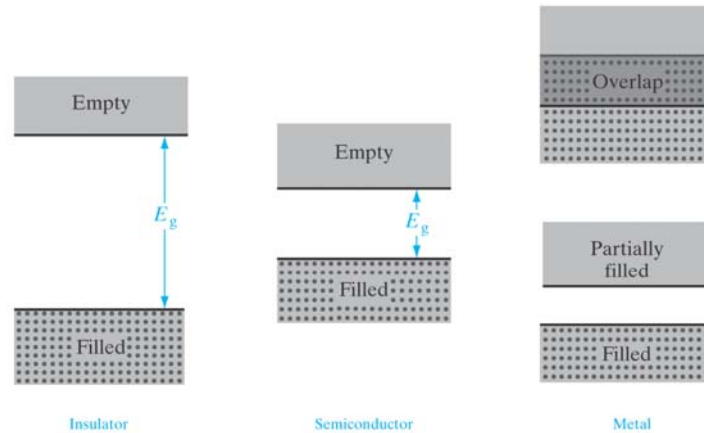


Figure 3.4

Typical band structures at 0 K.

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Semiconductor Materials

- Resistivities of materials used in solid state devices cover wide extremes.
 - Conductors: resistivity $<10^{-2} \Omega\text{-cm}$
 - Aluminum $<10^{-6} \Omega\text{-cm}$
 - Resistors: resistivity $>10^5 \Omega\text{-cm}$
 - Insulators:
 - Silicon Dioxide $\sim 10^{16} \Omega\text{-cm}$
 - Plastics in packaging $\sim 10^{18} \Omega\text{-cm}$
- Semiconductors have intermediate resistivities.
 - Resistivity can be widely varied.

Practical (3D) bands

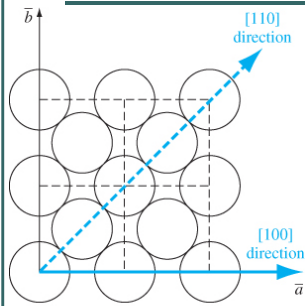


Figure 3.24 | The (100) plane of a face-centered cubic crystal showing the [100] and [110] directions.

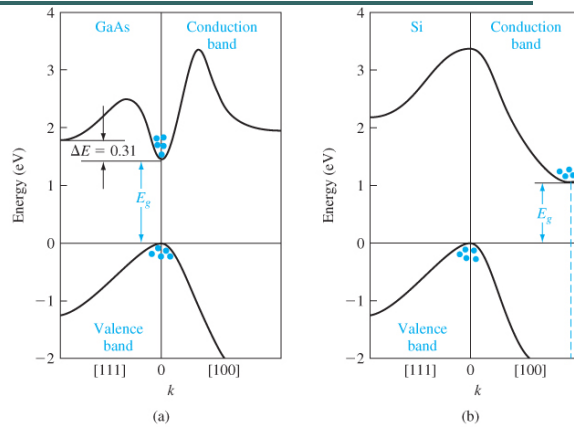


Figure 3.25 | Energy-band structures of (a) GaAs and (b) Si. (From Sze [12].)

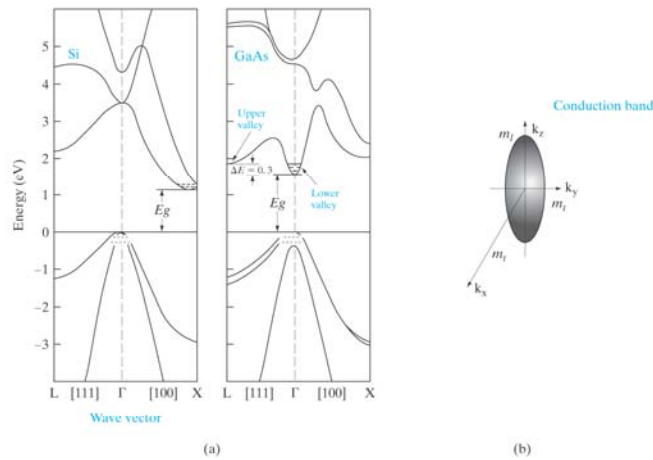
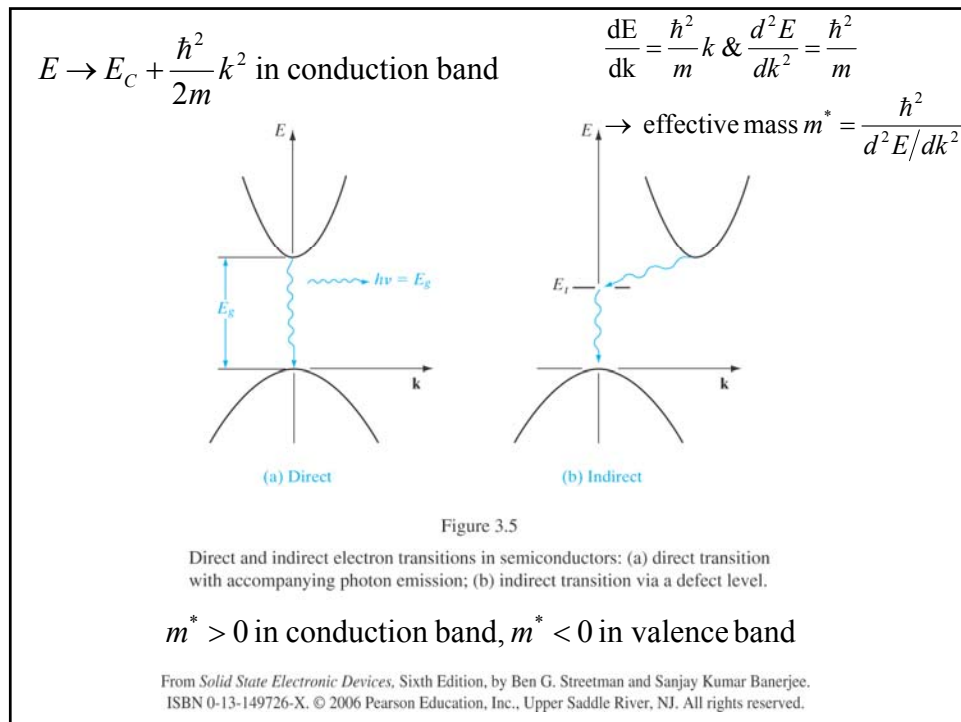


Figure 3.10

Realistic band structures in semiconductors: (a) Conduction and valence bands in Si and GaAs along [111] and [100]; (b) ellipsoidal constant energy surface for Si, near the 6 conduction band minima along the X directions. (From Chelikowsky and Cohen, Phys. Rev. B14, 556, 1976).

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Direct and Indirect Semiconductors

- When more exact quantum mechanical calculations are done the energy levels can be plotted against the propagation vector \mathbf{k} (aka wave-vector).
- $(\hbar\mathbf{k})$ is like particle momentum, which is = ??
- In direct semiconductors like GaAs the minimum of the conduction band and the maximum of the valence band occur at the same \mathbf{k} value ($\mathbf{k}=0$.)
- In indirect semiconductors like silicon the valence band max is at a different \mathbf{k} value.
 - A transition between bands requires a change in \mathbf{k} value (momentum) and is therefore less likely.
 - Usually done via a defect level.

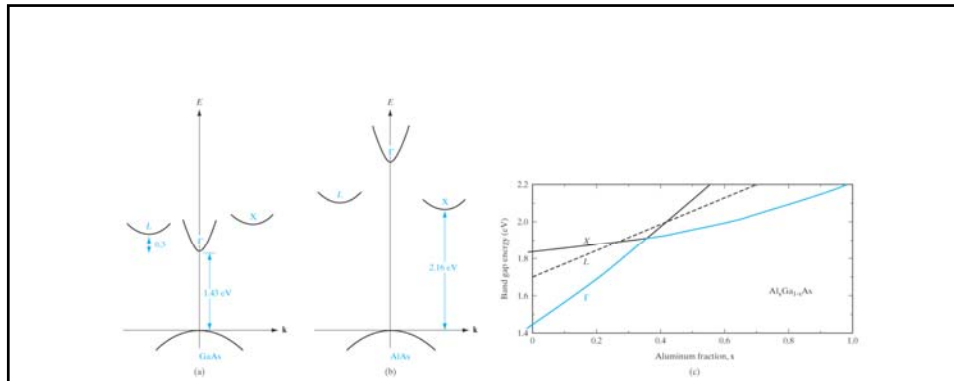


Figure 3.6

Variation of direct and indirect conduction bands in AlGaAs as a function of composition: (a) the (E, k) diagram for GaAs, showing three minima in the conduction band; (b) AlAs band diagram; (c) positions of the three conduction band minima in $Al_xGa_{1-x}As$ as x varies over the range of compositions from GaAs ($x = 0$) to AlAs ($x = 1$). The smallest band gap, E_g (shown in color), follows the direct Γ band to $x = 0.38$, and then follows the indirect X band.

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Extrinsic

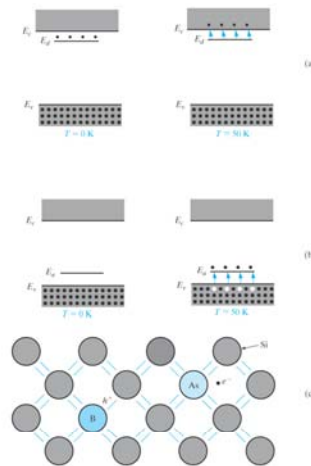


Figure 3.12

Energy band model and chemical bond model of dopants in semiconductors: (a) donation of electrons from donor level to conduction band; (b) acceptance of valence band electrons by an acceptor level, and the resulting creation of holes; (c) donor and acceptor atoms in the covalent bonding model of a Si crystal.

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Electron orbit around donor impurity

$$r_n = n^2 \frac{K^2 \hbar^2}{mq^2} \quad \& \quad K = 4\pi\epsilon_r\epsilon_0$$

For Si: $m^* = 0.26m_0$ & $\epsilon_r = 11.8$

For $n = 1$: $r_1 = 2.41nm \approx 4a$ for $a = 0.543nm$

i.e. orbit encompasses many lattice atoms

i.e. essentially free due to shielding effects
and lattice vibrations (phonons)

Today's Questions

- What are the different types of solids?
 - *Crystalline, amorphous, polycrystalline or*
 - *Semiconductor, metal, insulator.*
- What influences the arrangement?
 - *The outer shell electrons.*
 - *What states are available and occupied.*
- Why are the states in a solid different from those in isolated atoms or molecules?
 - *Pauli exclusion principle allows only one electron per state.*
- Why are two electrons allowed in an S-shell then?
 - *Electron spin up and spin down*

Questions

- How do these states change when a large number of atoms are brought together?
 - They must split into multiple states so that only one electron will be in each state.
 - There are so many of these states that they appear to be a continuum, or a band of available energies.
- How does that arrangement influence the electrical characteristics of the material? What band configuration makes an insulator or semiconductor?
 - Insulators and semiconductors have a valence band and a conduction band separated by a band gap.

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Questions

- What is the difference in band structure between a semiconductor and an insulator?
 - Semiconductors have smaller band gaps ($\sim 1\text{eV}$) so are more likely to experience thermal or optical excitation into the conduction band.
- What do the energy bands of a metal look like?
 - Bands overlap to provide a continuum with no energy gap, i.e. no distinction between valence and conduction electrons, and
 - Conduction band is partially filled at non-zero temperatures.

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Questions

- How many states are available in the outer shell?
How many are filled?
 - 8 states available (2 s and 6 p). 4 are filled with electrons.
- What kind of orbitals result from this configuration?
How are they arranged in space?
 - sp^3 hybrid orbitals. Four orbitals arranged in a tetrahedron.
- What kind of crystal structure results?
 - Diamond. Looks like two interpenetrating FCC lattices.

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Questions

- What is the electronic configuration of a metal?
How does that lead to good conductivity?
 - Outer shells only partially filled. Electrons easily given up and not tied to a particular atom.
- How does ionic bonding affect the electrical characteristics?
 - The transfer of electrons leads to effective charge on the ions and complete shells. So electrons are tightly bound and not available for conduction.

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Assignment #1

1. 1.8
2. 1.27
3. 2.7
4. 3.1
5. 3.12
6. 3.18
7. 3.19
8. 3.21