

Theory of Semiconductor Devices (반도체 소자 이론)

Lecture 8

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Tight Bound Electron Model

- In the **nearly free electron model** it was assumed that the **kinetic energy** of the electrons was **large** compared to the **periodic potential energy** due to the lattice.
- Under these conditions the **wavefunctions** were found to be **plane waves with a perturbation from the lattice**, and the **allowed energy bands** were **large** compared to the **forbidden energy regions**.
- In the **tightly bound electron model** this situation is **reversed**.
- The **periodic potential energy** due to the lattice is assumed to be **large** compared to the **kinetic energy** of the electrons, so that the **electrons are largely bound to the atomic cores**.
- In this situation we expect the electron **wavefunctions to be more like atomic orbitals** than plane waves.
- That is, we expect the **wavefunction overlap** between adjacent atoms in the lattice to be **sufficiently small** that the band structure will be closely related to the wavefunctions and **discrete energies** of electrons in **isolated atoms**.

Tight Bound Electron Model

- In this manner we consider N **isolated atoms** with electron wavefunctions ψ_a and **discrete energy levels** \mathcal{E}_a located at the lattice sites \mathbf{R} . The **one electron Schrödinger equation** for these **atoms** is

$$\mathbf{H}_a \psi_a(\mathbf{r} - \mathbf{R}) = \mathcal{E}_a \psi_a(\mathbf{r} - \mathbf{R}) \quad (2.83)$$

where

$$\mathbf{H}_a = -\frac{\hbar^2}{2m} \nabla^2 + U_a(\mathbf{r} - \mathbf{R}) \quad (2.84)$$

The **Bloch electrons** satisfy (2.1):

$$\mathbf{H} \psi_k(\mathbf{r}) = \mathcal{E} \psi_k(\mathbf{r}) \quad (2.85)$$

where

$$\mathbf{H} = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \quad (2.86)$$

and $U(\mathbf{r})$ satisfies (2.9).

$$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R}) \quad (2.9)$$

Tight Bound Electron Model

- We construct a wavefunction for the Bloch electrons from a *linear combination of atomic orbitals* (L.C.A.O.).

$$\psi_k(\mathbf{r}) = \sum_{\mathbf{R}} \exp(i\mathbf{k} \cdot \mathbf{R}) \psi_a(\mathbf{r} - \mathbf{R}) \quad (2.87)$$

which must satisfy **Bloch's theorem** (2.13). From (2.87) we have

$$\begin{aligned} \psi_k(\mathbf{r} + \mathbf{R}') &= \sum_{\mathbf{R}} \exp(i\mathbf{k} \cdot \mathbf{R}) \psi_a(\mathbf{r} + \mathbf{R}' - \mathbf{R}) \\ &= \exp(i\mathbf{k} \cdot \mathbf{R}') \sum_{\mathbf{R}} \exp[i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')] \psi_a[\mathbf{r} - (\mathbf{R} - \mathbf{R}')] \\ &= \exp(i\mathbf{k} \cdot \mathbf{R}') \psi_k(\mathbf{r}) \end{aligned} \quad (2.88)$$

which is Bloch's theorem.

- The Bloch electron Hamiltonian (2.86) can be put in the form

$$\begin{aligned} \mathbf{H} &= -\frac{\hbar^2}{2m} \nabla^2 + U_a(\mathbf{r} - \mathbf{R}) + \Delta U(\mathbf{r} - \mathbf{R}) \\ &= \mathbf{H}_a + \Delta U(\mathbf{r} - \mathbf{R}) \end{aligned} \quad (2.89)$$

Tight Bound Electron Model

where

$$\Delta U(\mathbf{r} - \mathbf{R}) \equiv U(\mathbf{r}) - U_a(\mathbf{r} - \mathbf{R}) \quad (2.90)$$

indicates the extent to which the periodic potential energy of the crystal deviates from the isolated atomic potential (Fig. 2.9). If the electrons are *tightly bound*, this deviation is *small*.

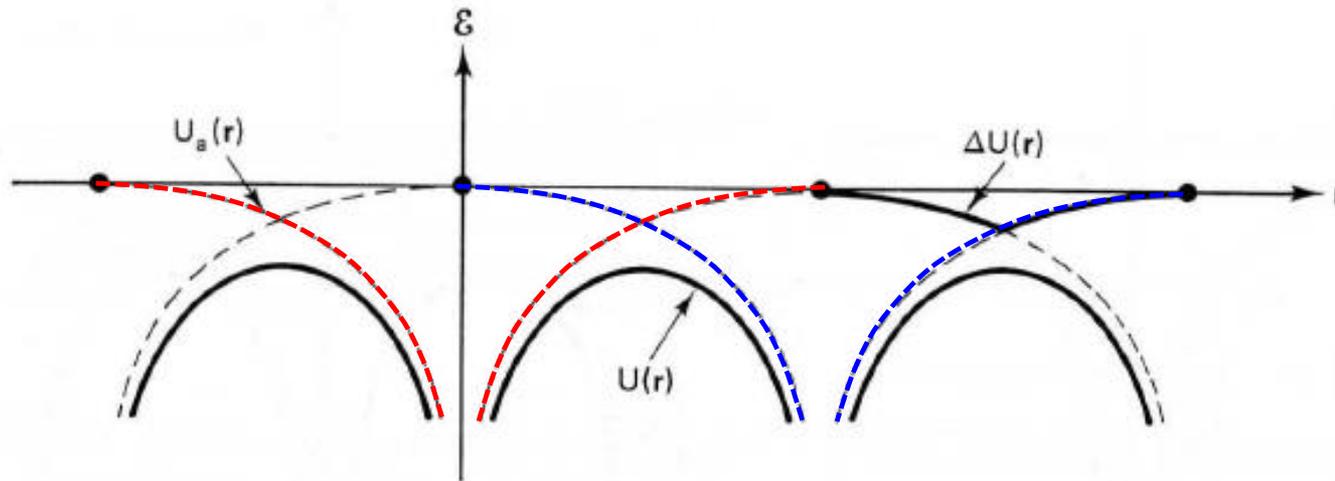


Figure 2.9 The periodic lattice potential energy, atomic potential energies, and their difference for \mathbf{r} in the direction of \mathbf{R} .

Tight Bound Electron Model

- Operating on (2.87) with (2.84), we find that

$$\begin{aligned}
 \mathbf{H}_a \psi_k(\mathbf{r}) &= \left[-\frac{\hbar^2}{2m} \nabla^2 + U_a(\mathbf{r} - \mathbf{R}) \right] \sum_{\mathbf{R}} \exp(i\mathbf{k} \cdot \mathbf{R}) \psi_a(\mathbf{r} - \mathbf{R}) \\
 &= \sum_{\mathbf{R}} \exp(i\mathbf{k} \cdot \mathbf{R}) \mathbf{H}_a \psi_a(\mathbf{r} - \mathbf{R}) \\
 &= \mathcal{E}_a \psi_k(\mathbf{r})
 \end{aligned} \tag{2.91}$$

- Using (2.89) in (2.85), we have

$$\mathcal{E} \psi_k(\mathbf{r}) = [\mathbf{H}_a + \Delta U(\mathbf{r} - \mathbf{R})] \psi_k(\mathbf{r}) \tag{2.92}$$

$$(\mathcal{E} - \mathcal{E}_a) \psi_k(\mathbf{r}) = \Delta U(\mathbf{r} - \mathbf{R}) \psi_k(\mathbf{r}) \tag{2.93}$$

- Multiplying on the left by $\psi_k^*(\mathbf{r})$ and **integrating over the crystal volume** yields

$$(\mathcal{E} - \mathcal{E}_a) \int_V \psi_k^*(\mathbf{r}) \psi_k(\mathbf{r}) d\mathbf{r} = \int_V \psi_k^*(\mathbf{r}) \Delta U(\mathbf{r} - \mathbf{R}) \psi_k(\mathbf{r}) d\mathbf{r} \tag{2.94}$$

- Since the wavefunctions are **normalized over the volume of the unit cell Ω** , the integral on the left-hand side of (2.94) is just equal to the **number of atoms in the crystal**,

$$\mathcal{E} - \mathcal{E}_a = \frac{1}{N} \int_V \psi_k^*(\mathbf{r}) \Delta U(\mathbf{r} - \mathbf{R}) \psi_k(\mathbf{r}) d\mathbf{r} \tag{2.95}$$

Tight Bound Electron Model

- We now substitute the *atomic* wavefunctions of (2.87) for the *Bloch* wavefunctions in (2.95), with the result

$$\mathcal{E} - \mathcal{E}_a = \frac{1}{N} \sum_{\mathbf{R}} \sum_{\mathbf{R}'} \exp [i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')] \int_V \psi_a^*(\mathbf{r} - \mathbf{R}') \Delta U(\mathbf{r} - \mathbf{R}) \psi_a(\mathbf{r} - \mathbf{R}) d\mathbf{r} \quad (2.96)$$

- Because of the *periodicity* of the lattice, we can *set the origin at \mathbf{R}* for each term in the summation over \mathbf{R} (set $\mathbf{R} = 0$). It is then easy to see that all N terms in the summation over \mathbf{R} are identical and (2.96) becomes

$$\mathcal{E} - \mathcal{E}_a = \sum_{\mathbf{R}'} \exp (-i\mathbf{k} \cdot \mathbf{R}') \int_V \psi_a^*(\mathbf{r} - \mathbf{R}') \Delta U(\mathbf{r}) \psi_a(\mathbf{r}) d\mathbf{r} \quad (2.97)$$

If we take out the term for $\mathbf{R}' = 0$, we have

$$\mathcal{E} = \mathcal{E}_a - \alpha - \sum_{\mathbf{R}' \neq 0} \beta_{\mathbf{R}'} \exp (i\mathbf{k} \cdot \mathbf{R}') \quad \text{for } \mathbf{R}' \neq 0 \quad (2.98)$$

where

$$\alpha \equiv - \int_V \psi_a^*(\mathbf{r}) \Delta U(\mathbf{r}) \psi_a(\mathbf{r}) d\mathbf{r} \quad (2.99)$$

$$\beta_{\mathbf{R}'} \equiv - \int_V \psi_a^*(\mathbf{r} - \mathbf{R}') \Delta U(\mathbf{r}) \psi_a(\mathbf{r}) d\mathbf{r} \quad (2.100)$$

and \mathbf{R}' is now a vector joining an atom at the origin to all other atoms in the crystal. Since the integrals in (2.99) and (2.100) are difficult to calculate, we will express our results in terms of α and $\beta_{\mathbf{R}'}$

Tight Bound Electron Model

- In (2.98) α is referred to as the **Coulomb energy**. It determines the **shift** in the atomic core levels, \mathcal{E}_a , caused by the **interactions among atoms**. $\beta_{R'}$ is referred to as the **exchange energy** and it **determines the extent of broadening of the atomic levels into energy bands** (Fig. 2.10).
- Since $\Delta U(\mathbf{r})$ is **negative** and becomes larger with decreasing atomic spacing, both α and $\beta_{R'}$ are **positive** and increase in magnitude with decreasing atomic spacing.

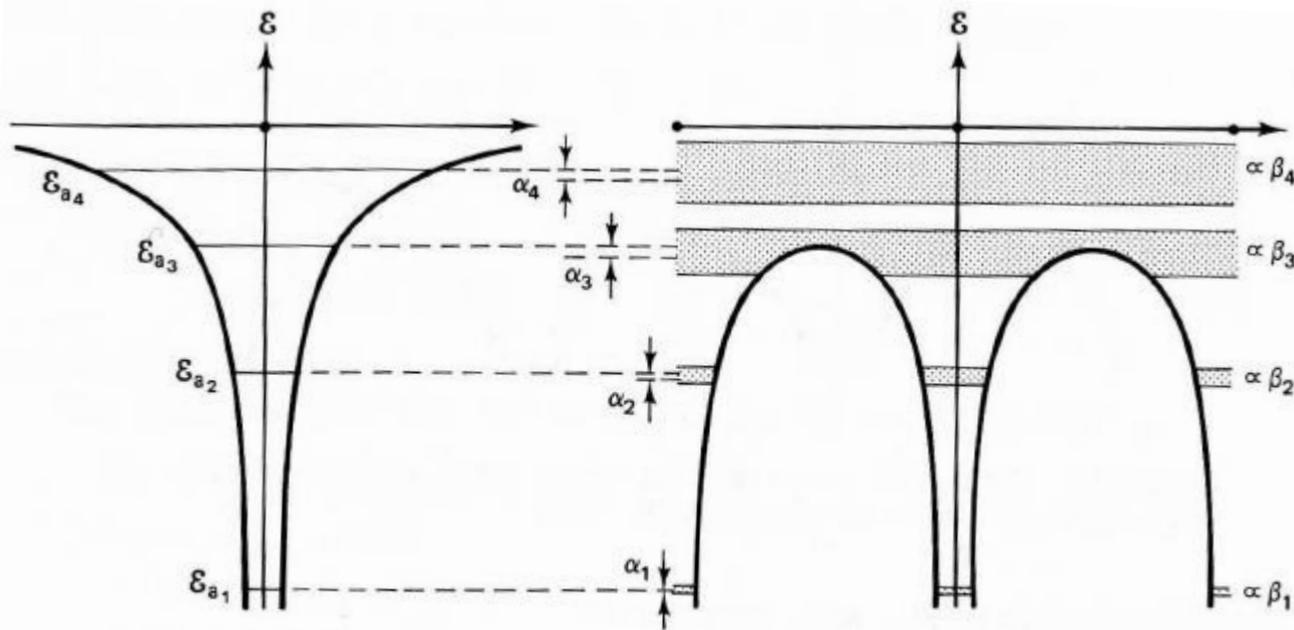


Figure 2.10 Diagram showing how energy bands are formed from the terms in (2.98). Each band is constructed from one atomic level.

Tight Bound Electron Model

- Thus these terms contain the **overlap of atomic orbitals** and account for the difference in potential energy between **isolated atoms** and a **crystal** of interacting atoms. The series in (2.98) allows for a summation of the overlap between an atom at the origin and all other atoms in the crystal. From Fig. 2.9, however, it can be seen that most of $\Delta U(\mathbf{r})$ can be accounted for by **summing over nearest-neighbor atoms only**.
- As an example, let us consider the tight-binding energy bands for a **face-centered cubic** direct lattice with a basis of one atom. For spherically symmetric atomic wavefunctions, $\beta_{R'} = \beta$ is the **same for all nearest neighbors**. Figure 2.11 shows that there are 12 nearest neighbors in this structure located at

$$\mathbf{R} = \frac{a}{2} (\pm \hat{x} \pm \hat{y}),$$

$$\frac{a}{2} (\pm \hat{y} \pm \hat{z}),$$

$$\frac{a}{2} (\pm \hat{x} \pm \hat{z})$$

(2.101)

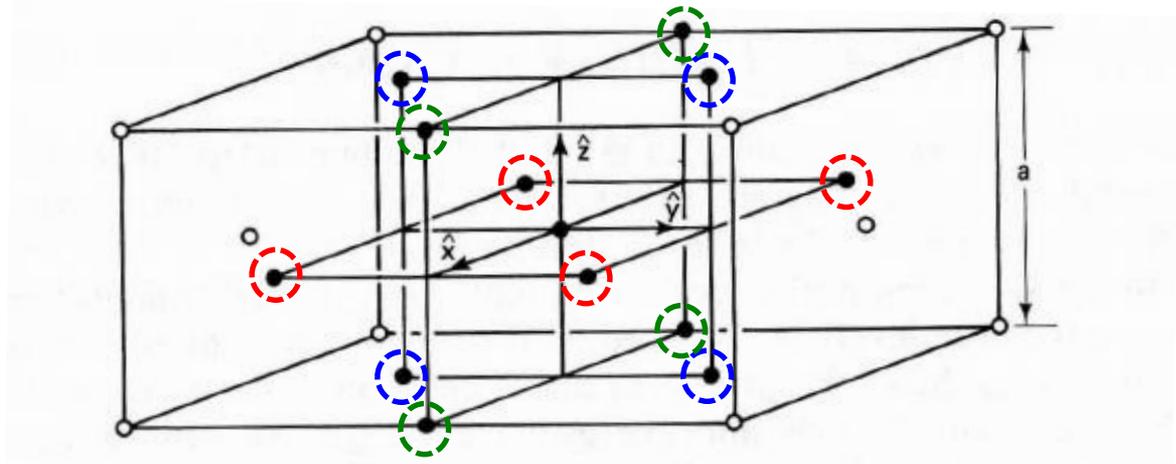


Figure 2.11 The 12 nearest-neighbor atoms (solid spheres) in face-centered cubic structure.

Tight Bound Electron Model

- For \mathbf{k} in the form

$$\mathbf{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z} \quad (2.102)$$

(2.98) becomes

$$\begin{aligned} \mathcal{E} = \mathcal{E}_a - \alpha - 4\beta [& \cos \frac{1}{2}k_x a \cos \frac{1}{2}k_y a + \cos \frac{1}{2}k_y a \cos \frac{1}{2}k_z a \\ & + \cos \frac{1}{2}k_z a \cos \frac{1}{2}k_x a] \quad (2.103) \end{aligned}$$

- Equation (2.103) shows that the **energy of a Bloch electron**, derived from one atomic state, consists of **some constant value** and an expression that varies with wavefunction **between well-defined limits**. Thus we find that for every electron state in the free atom, there exists a band of energies in the crystal.

- Figure 2.12 shows this **tight-binding energy band** for several **high-symmetry directions** in the first Brillouin zone. This figure can be compared directly to the lowest-lying **empty lattice energy band** in Fig. 2.6. It can be noted that the **width of the band depends on β** and varies for different directions of wave vector in a manner similar to the lowest-lying empty lattice band.

Tight Bound Electron Model

- This similarity shows the **strong** dependence of energy band structure on the crystal lattice. The number of **nondegenerate** electronic states in the band is equal to N , the number of atoms in the crystal, and **each state can be occupied by two electrons of opposite spin**. To obtain the complete energy band diagram in the tight-binding approximation, it is necessary to add **additional** atomic states to this picture, as indicated in Figs. 2.10 and 2.13.

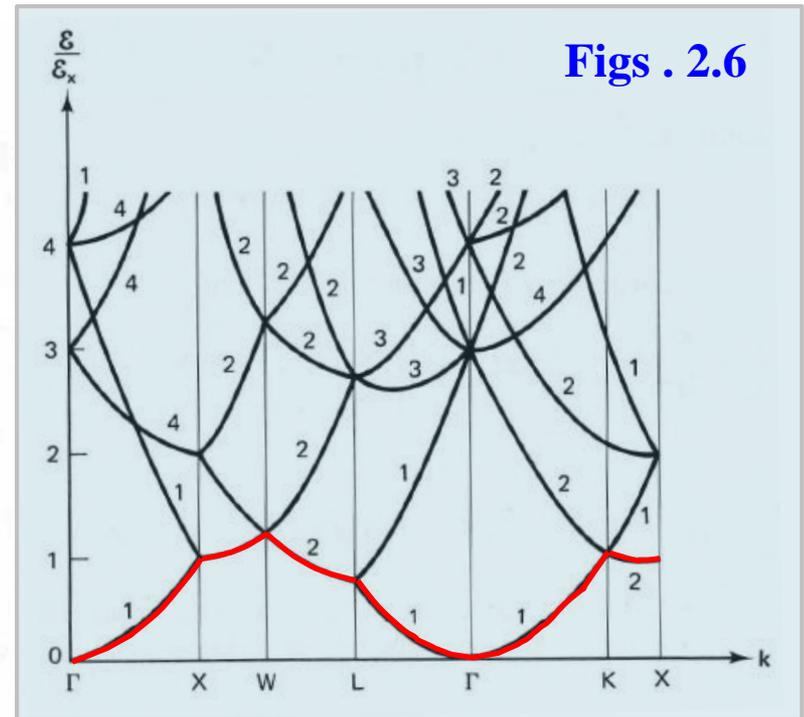
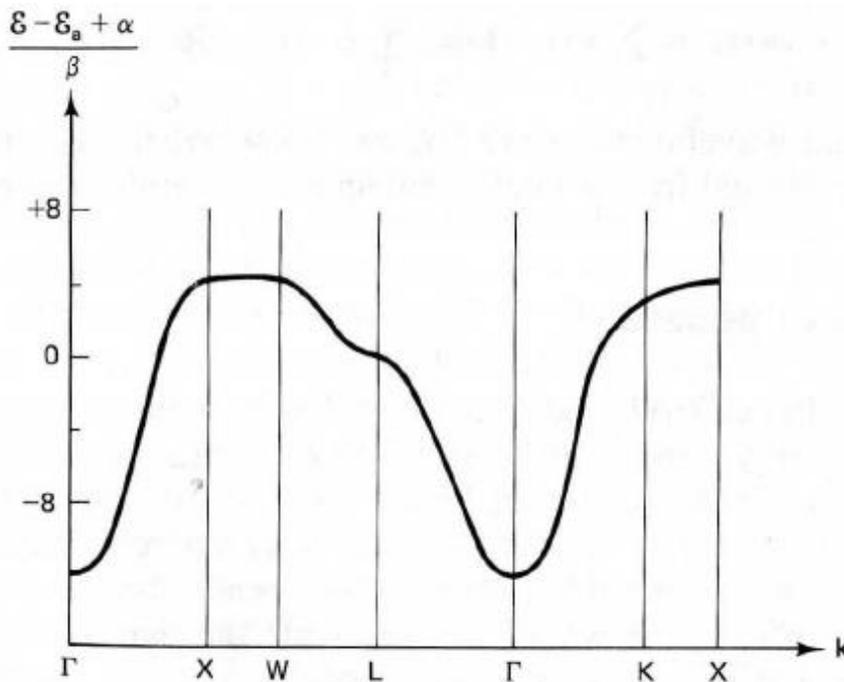


Figure 2.12 Tight-binding energy band, corresponding to one atomic state, for a face-centered cubic lattice with a basis of one atom.

Tight Bound Electron Model

- Figure 2.13 illustrates conceptually how the complete energy band diagram for a crystal can be obtained from discrete atomic levels. We take N atoms and locate them on the sites of the appropriate Bravais lattice, except that the distance between atoms is so *large* that they *do not interact*. Each atomic level is then *N -fold degenerate* (excluding spin and angular momentum degeneracy).

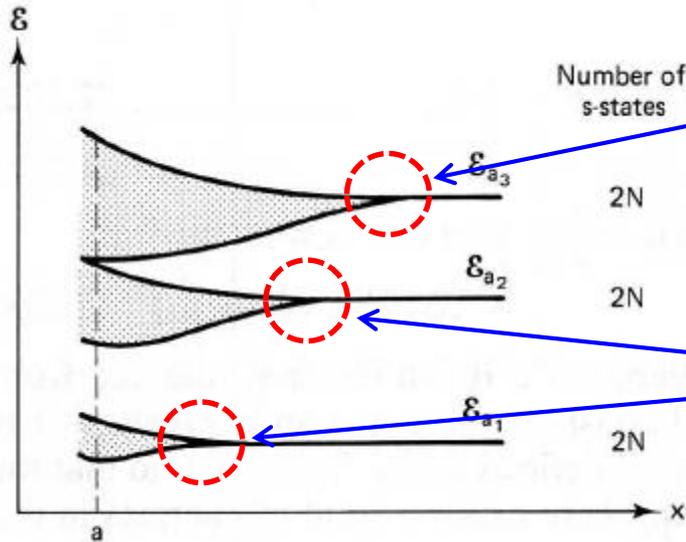


Figure 2.13 Diagram showing how energy bands in tightly bound electron model are formed from discrete atomic levels as the distance between atoms, x , is decreased to the lattice constant, a .

- As we bring the atoms closer together, the higher-energy atomic states begin to interact, because of their large orbitals, and the N degenerate states **split into a band of N discrete states**.

- As the distance between atoms decreases further, lower-lying atomic levels begin to split into bands, and so on.

- In this manner, band states can be **classified** according to their atomic origin. That is, bands can be referred to as *s*-bands, *p*-bands, and so on. For higher-lying bands that overlap, however, this classification is not as obvious.

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Other Band Models

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- Pseudopotential Method
- Cellular Methods
- Spin-Orbit Coupling

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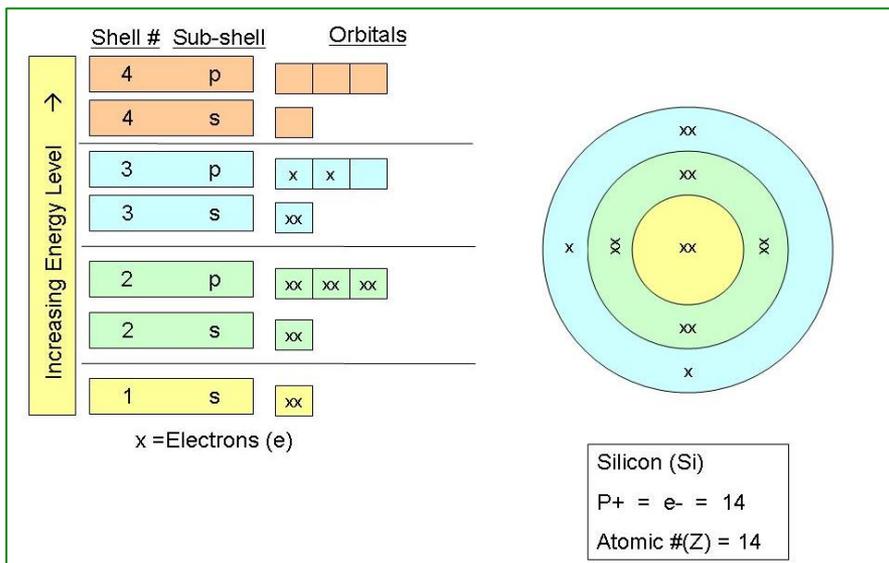
2.6 **Valence Bands and Bonds**

2.7 Energy Band Structure

2.8 Electron Dynamics

Valence Bands and Bonds

- Before we consider the details of semiconductor energy bands, it is worthwhile to pursue the **relationship between energy bands and valence bonds**.
- We learned in Section 2.1 that the **first Brillouin zone** for a direct Bravais lattice has N allowed values of k , where N is the number of primitive unit cells in the direct lattice. Each allowed k value corresponds to a wavefunction or electron state which can have **two electrons of opposite spin**.
- Including spin, we then have **$2N$ electron states per energy band** or **two electron states per unit cell per energy band** for a Bravais lattice.
- If we now add a **basis** (atoms) to the lattice to obtain a crystal structure, we can count the **number of electrons per unit cell** and determine the **occupancy** of the energy bands.



- As an example, let us consider the occupancy of energy bands in silicon.
- Silicon has the diamond crystal structure, which is a face-centered cubic Bravais lattice with a basis of two atoms per primitive unit cell.
- The atomic structure is

$$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^2.$$

Valence Bands and Bonds

- Since the **first two shells** are completely filled and *tightly bound* to the nucleus, we will consider only the third shell of **valence electrons**. Here the **two 3s states** (including spin states) are completely filled with two electrons, and the **six 3p states have only two electrons**.

- If we use a **tight-binding** approach to form the crystal from the atoms, we will need **2N silicon atoms**. As shown in Fig. 2.14, the resulting **12N 3p-states** and the **4N 3s-states** **interact and cross over** when the atoms are **brought together** to the appropriate lattice constant. The result for 0 K is **8N lower-lying states** occupied by **8N electrons** separated by an **energy gap** from **8N higher-lying states** with zero electrons.

- Since there are **2N states per energy band**, the crystal has three 3p bands and one 3s band (all **spin degenerate**) in both the low- and high-energy regions. The four bands appear to be only one in an \mathcal{E} versus r diagram, as in Fig. 2.14.

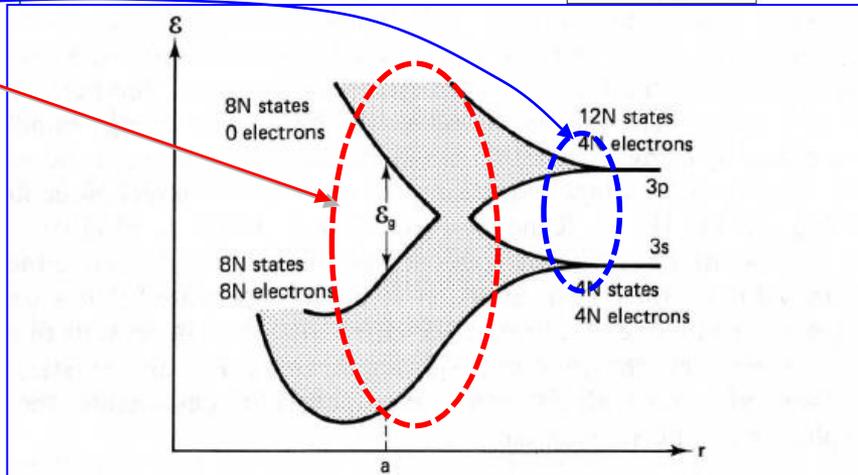
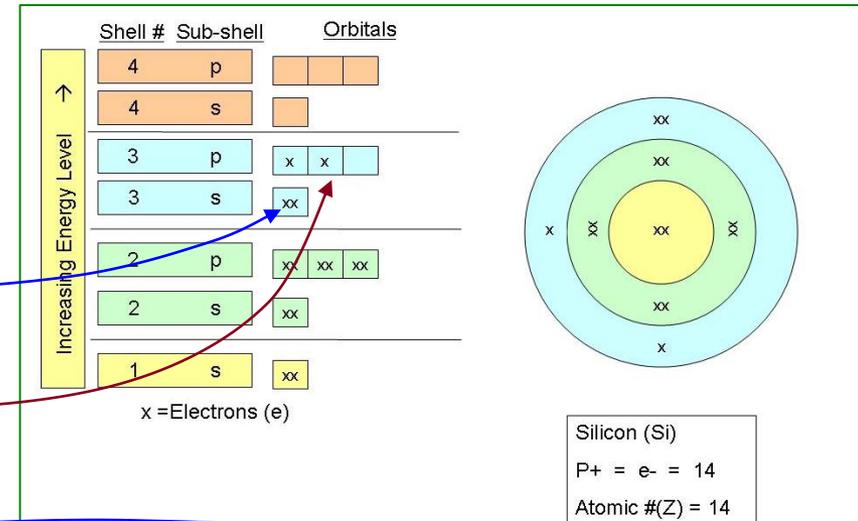
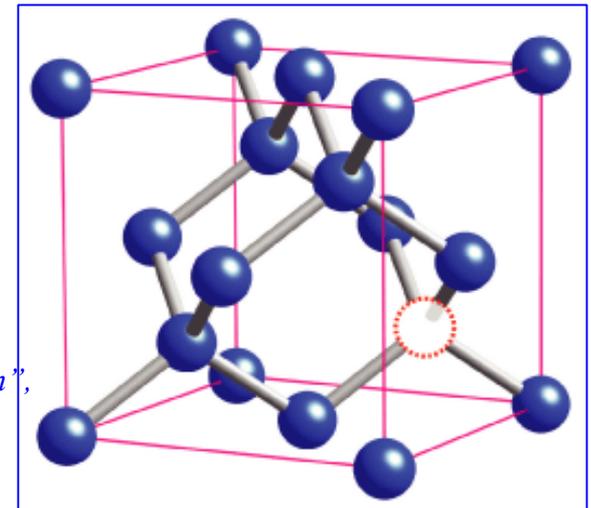


Figure 2.14 The formation of energy bands in silicon from the two-highest occupied atomic levels. The 8N available electrons completely fill the 8N states in the lowest bands (valence bands), leaving the 8N states in the highest bands (conduction bands) completely empty.

Valence Bands and Bonds

- In molecules such as CH_4 this combination of s and p states is known to give a tetrahedral bonding arrangement, called *covalent bonding*, where two electrons of opposite spin are shared between atoms.
- For the silicon crystal, however, there are $8N$ electrons in the four lower-lying bands, or **eight electrons per unit cell**. This means that every silicon atom in the crystal is surrounded by eight outer electrons. From the crystal structure of silicon (Fig. 1.10), we see that every silicon atom has **four nearest neighbors**, so that each silicon atom must be *covalently bonded* to its nearest neighbors, **with the $8N$ electrons** in the lowest-lying energy bands.
- For this reason these occupied bands are referred to as *valence bands*.
- The decrease in the energy of these bands over the atomic states, as shown in Fig. 2.14, reflects the binding or cohesive energy.
- In a similar manner the four higher-lying bands correspond to an antibonding molecular state and are referred to as *conduction bands*.



From "Semiconductor Device Physics and Design",
U. Mishra, J. Singh (Springer, 2008)

Valence Bands and Bonds

- It should be pointed out, however, that this analogy with covalently bonded molecules is not precise.
- The wavefunction overlap, which produces the energy bands in the crystal, demonstrates that the *valence electrons are not localized in the bonds*. There is, nevertheless, a high concentration of electron charge in the regions between atoms, which is equivalent to a covalent electron pair.

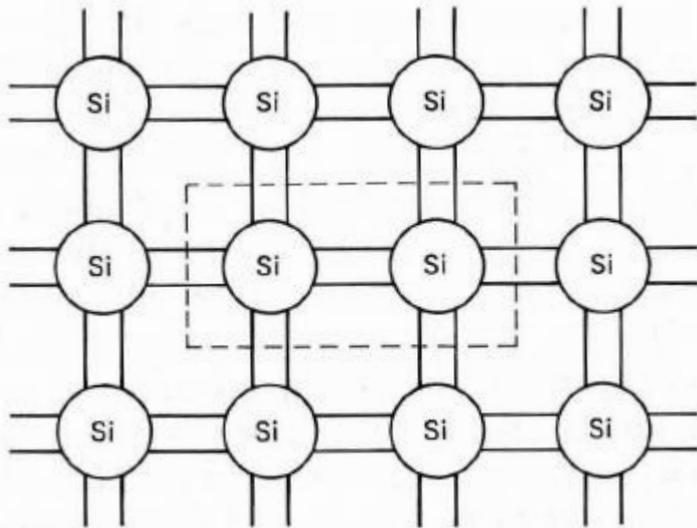
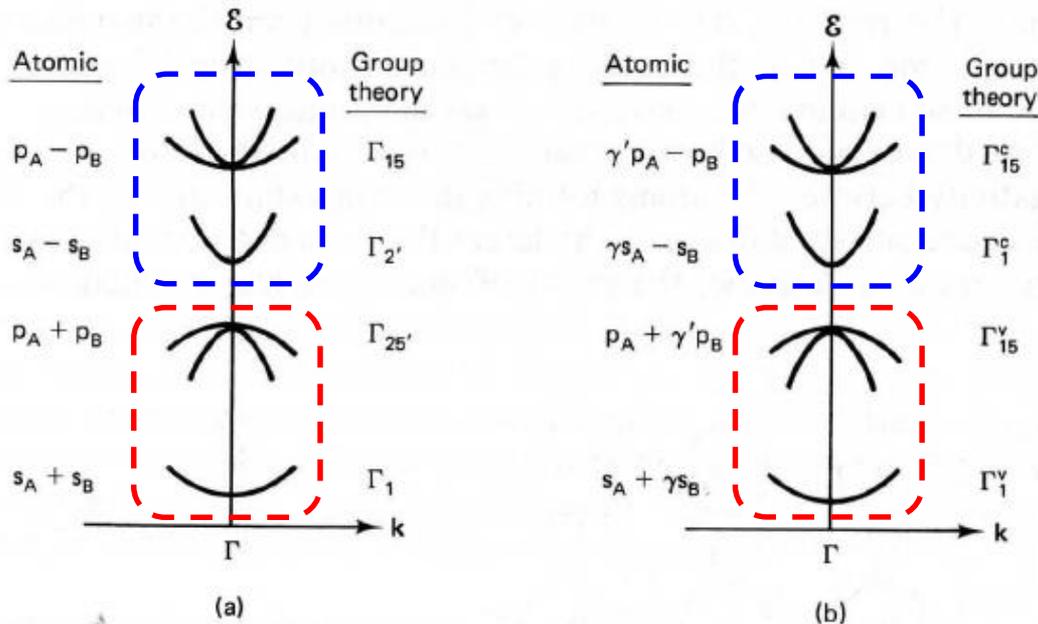


Figure 2.15 Two-dimensional schematic of covalent bonding arrangement in silicon. The dashed lines show the Wigner-Seitz unit cell.

- This covalent bonding arrangement can conveniently be illustrated by the **two-dimensional schematic** shown in Fig. 2.15. Each solid line between atoms represents one of the paired electrons in the covalent bond. Adding up the number of electrons in the Wigner-Seitz unit cell, we find a **total of eight**. These are the eight electrons that completely fill the four valence bands in Fig. 2.14.
- The other column IV semiconductors can be represented in a similar fashion.

Valence Bands and Bonds

- To illustrate the origin of the various bands, we can look at the \mathcal{E} versus \mathbf{k} curve near the Γ -point as in Fig. 2.16(a).
- The lowest-lying valence band, labeled Γ_1 , is twofold (spin) degenerate and is derived from the bonding s orbitals for the two atoms in the unit cell.
- The other three valence bands ($\Gamma_{25'}$) are derived from p orbitals and are sixfold degenerate



at Γ . When spin orbit effects are included, these bands are split into two fourfold degenerate bands, labeled $\Gamma_{25'}^{3/2}$, and one lower-lying twofold degenerate band, labeled $\Gamma_{25'}^{1/2}$, at r . These three valence bands are also referred to as the **heavy mass**, **light mass**, and **split-off bands**, in order of decreasing energy.

- As indicated in Fig. 2.16, the **four conduction bands** are derived from antibonding s and p orbitals, with properties that reflect these atomic states.

Figure 2.16 Tight-binding prescription near Γ for the conduction and valence bands of crystals with (a) the diamond structure and (b) the sphalerite structure. The eight bands are labeled with both atomic and group theory notation. Spin-orbit coupling effects are neglected. A and B refer to the two atoms in the unit cell.

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Energy Band Structures

- Figure 2.18 shows the results of an empirical pseudopotential calculation for the energy bands of the elemental semiconductors **Si** and **Ge**. The results of this calculation are in good agreement with experiments, except that spinorbit effects are not included. These materials have the diamond crystal structure.

- As can be seen, the $\Gamma_{25'}$ valence bands for these two materials are quite similar, with the maximum at the Γ -point. The Γ_1 -band is off-scale on the lower end of these figures. Although the valence bands are similar, there are significant differences in the conduction band structure.

-For many applications the most important energy band parameter is the energy gap, \mathcal{E}_g , defined as the minimum separation between the conduction and valence bands.

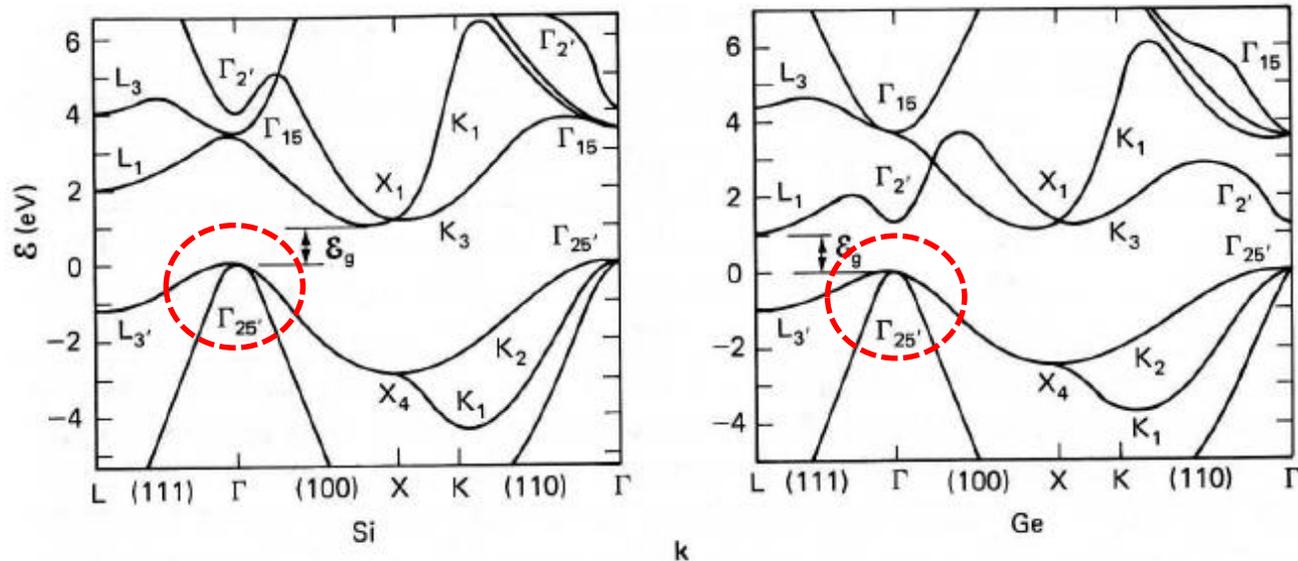
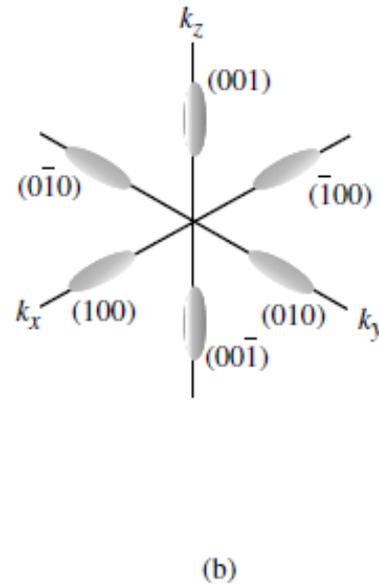
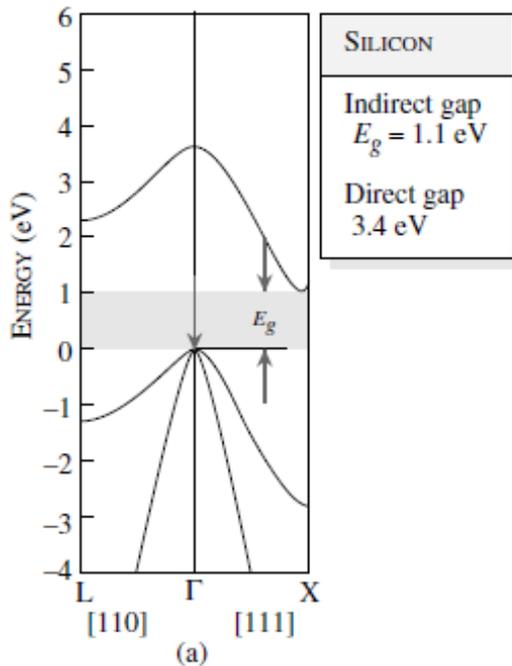


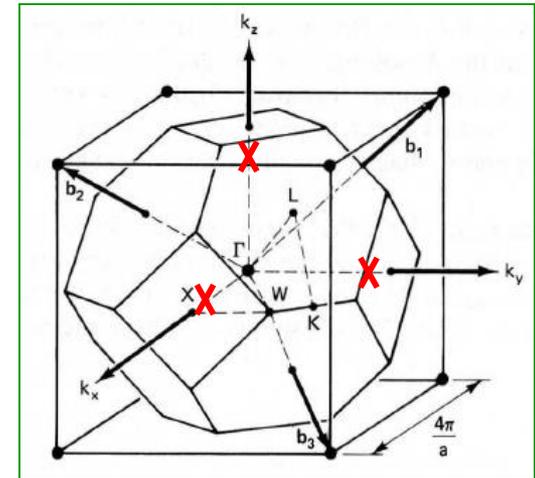
Figure 2.18 Empirical pseudopotential results for the energy bands of the elemental semiconductors Si and Ge. [After M. L. Cohen and T. K. Bergstresser, *Phys. Rev.* 141, 789 (1966).]

Energy Band Structures

- For Si the energy gap (1.17 eV at 0 K) is between the valence band maximum at Γ and the conduction band minimum at about 0.8X in the (100) direction.
- This energy gap is referred to as an *indirect bandgap*, since a change in \mathbf{k} value is required for an electron to make a transition from this conduction band minimum to the valence band maximum.
- Also, we note that there are six {100} directions in reciprocal space, so that the minimum at 0.8X in Si is actually *six equivalent minima*.



Constant energy surfaces of six equivalent valleys at conduction band edge



(a) Band structure of Si.
(b) Constant energy ellipsoids for the Si conduction band. There are *six equivalent valley* in Si at the band edge.

Energy Band Structures

- Most of the III-V compound semiconductors have the **sphalerite** crystal structure , so we expect the form of the energy bands to be similar to those for the diamond structure.
- The energy bands for **GaAs** and **GaP**, shown in Fig. 2.19, are fairly typical of this class of materials.
- As can be seen, the valence band structures are quite similar to Si and Ge. The minimum conduction band energy for GaP is at the X-point, so that **GaP** has an **indirect bandgap** with three equivalent conduction band minima.
- **GaAs**, however, has a minimum in the conduction band at Γ . Since no change in \mathbf{k} value is required for an electron to go from this conduction band to the maximum in the valence band, GaAs has a **direct bandgap**.

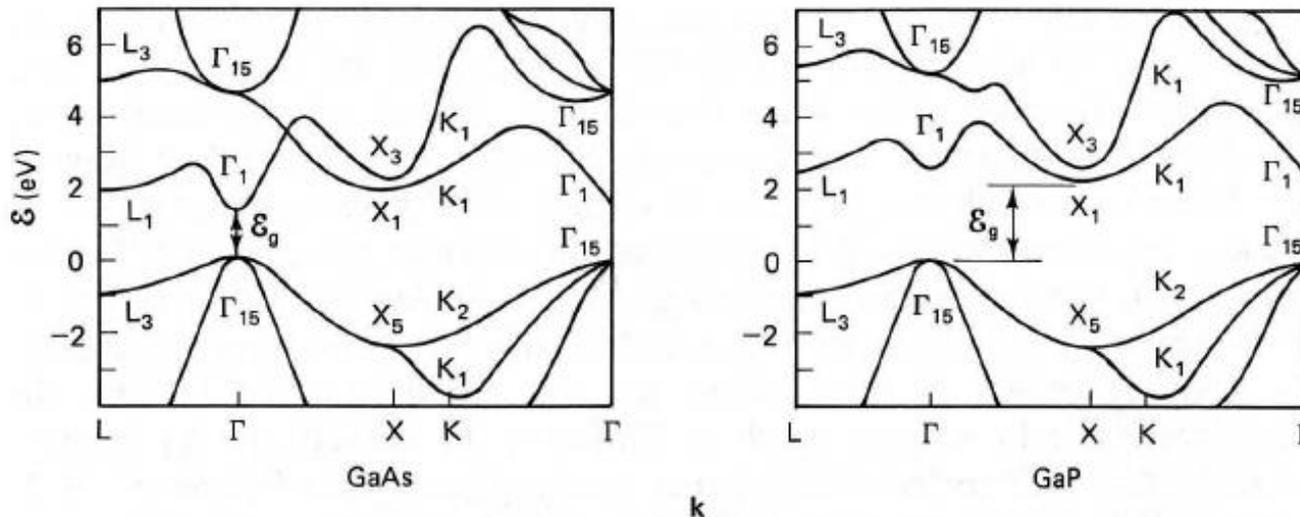


Figure 2.19

Energy bands for the 111-V compound semiconductors GaAs and GaP.
[After M. L. Cohen and T. K. Bergstresser, *Phys. Rev.* 141 , 789 (1966).]

Valence Bands

- In the energy band calculations above, **spin-orbit effects** are not included.
- When these effects are taken into account, some of the **degeneracy of the highest-lying valence bands is removed**, resulting in a **lower split-off band**.
- The energy separation between this split-off band and the degenerate light- and heavy-hole bands is referred to as the **spin-orbit energy, Δ** , shown in Fig. 2.23. Values of this parameter for a number of semiconductors are listed in Table 2.3.

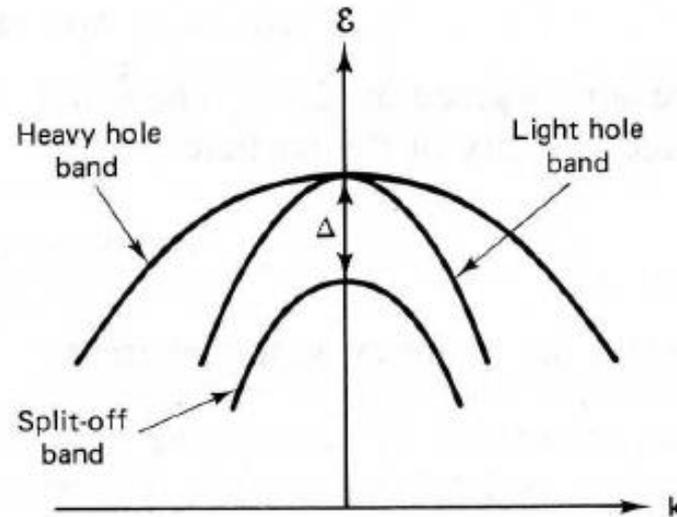


Figure 2.23 Heavy-hole, light-hole, and split-off valence bands.

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Electron Dynamics

- There is an **intimate relationship** between **band structure** and the **transport properties of electrons**. By **transport properties** we mean the **response of the electrons to applied forces**.
- The proper approach to the problem of electronic motion in a periodic lattice would be to solve the time-dependent Schrodinger equation.
- A simpler solution, however, can be obtained, by first constructing a **wave packet** from plane wave solutions to the **time-dependent Schrodinger equation**. Then since it is well known that this wave packet behaves as a classical particle (correspondence principle) , we can treat the problem **semiclassically**.
- Let us then construct a **wave packet (particle)** from solutions to the time-dependent equation of the form

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp(-i\omega t) \quad (2.105)$$

where $\psi(\mathbf{r})$ is given in (2.10). The group velocity of the wave packet (or the average velocity of the particle) is

$$\mathbf{v} = \nabla_{\mathbf{k}} \omega = \frac{\partial \omega}{\partial \mathbf{k}} \quad (2.106)$$

Electron Dynamics

- If we use the quantum scalar operator

$$\mathcal{E} \equiv -\frac{\hbar}{i} \frac{\partial}{\partial t} \quad (2.107)$$

on the wave packet formed from (2.105), we obtain

$$\mathcal{E} = \hbar\omega \quad (2.108)$$

which is just Planck's relationship. With this, (2.106) becomes

$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E} = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \mathbf{k}} \quad (2.109)$$

- It should be pointed out that (2.109) is a rather **surprising** result. It tells us that an electron in a **state specified by wave vector \mathbf{k}** in a **given energy band** has a **velocity determined by the slope of the \mathcal{E} versus \mathbf{k} curves**. An examination of the \mathcal{E} versus \mathbf{k} diagrams in Section 2.7 shows that for most allowed values of \mathbf{k} , the electrons will have a finite velocity.

- Thus an electron moving in a **perfect periodic potential** with **no applied forces** has a constant velocity and is **not scattered** by the atoms of the crystal. In other words, **a perfect crystal offers no resistance to the motion of an electron**. Only crystal **imperfections serve to scatter electrons**.

- We examine these scattering processes in Chapter 6.

Effective Mass

- In the meantime, let us apply an external force \mathbf{F} to the wave packet. This force changes the energy of the electron according to

$$\mathbf{v} \cdot \mathbf{F} = \frac{d\mathcal{E}}{dt} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E} \cdot \hbar \frac{d\mathbf{k}}{dt} \quad (2.110)$$

Then from (2.109),

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F} \quad (2.111)$$

$$\mathbf{p}\psi_{\mathbf{k}}(\mathbf{r}) = \hbar\mathbf{k}\psi_{\mathbf{k}}(\mathbf{r}) + \exp(i\mathbf{k} \cdot \mathbf{r}) \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

- This is an important relationship. It tells us that $\hbar\mathbf{k}$ behaves as a **momentum for external forces applied to a Bloch electron**. It is for this reason that we defined a **crystal momentum** in (2.32).

- Let us now take the time **derivative of the velocity** in (2.109), to get

$$\frac{d\mathbf{v}}{dt} = \frac{1}{\hbar} \frac{d}{dt} \nabla_{\mathbf{k}} \mathcal{E} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \left[\nabla_{\mathbf{k}} \mathcal{E} \cdot \frac{d\mathbf{k}}{dt} \right] \quad (2.112)$$

Using (2.111), equation (2.112) becomes

$$\mathbf{a} = \frac{1}{\hbar^2} \nabla_{\mathbf{k}} [\nabla_{\mathbf{k}} \mathcal{E} \cdot \mathbf{F}] \quad (2.113)$$

where \mathbf{a} is the electron acceleration.

Effective Mass

- This equation tells us that \mathbf{F} can produce a change in \mathbf{v} in directions other than the direction of \mathbf{F} . Comparing this to the Newtonian force equation, we see that the closest thing to a mass for the electron is an inverse tensor which depends on the curvature of the \mathcal{E} versus \mathbf{k} diagrams. This can be determined by resolving (2.113) into components along three arbitrary axes. Then

$$a_i = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 \mathcal{E}}{\partial k_i \partial k_j} F_j \quad \text{for } i, j = 1, 2, 3 \quad (2.114)$$

and we obtain an **inverse effective mass tensor** with components

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k_i \partial k_j} \quad (2.115)$$

-If we examine the **curvature** of some of the energy bands in Section 2.7, we see that **at band minima the effective mass is positive** and **at band maxima the effective mass is negative**. This is the same as the result that we found for the nearly free electron energy bands in Section 2.3.

- Another conclusion that results from (2.115) is that the **effective mass becomes infinite at some point within a band**. This merely indicates the point in the band where the externally applied force stops accelerating and begins decelerating the electron.

- From (2.115) we can also see why the $\Gamma_{25'}$ and Γ_{15} valence bands in Figs. 2.18 and 2.19, respectively, are referred to as light and heavy bands.