- Band structure in semiconductors:
 - Direct/indirect bandgaps
 - Density of states
 - Electrons and Holes
- E-k relationships for:
 - Silicon
 - GaAs
 - Germanium

1

Reminder of Lecture 1 Concepts



Band structure of semiconductors

- A solution of the Schrödinger equation provides an energy versus effective momentum E-k relationship. This is called the **band structure** of the semiconductor.
- In semiconductor physics, we are interested in the properties of the E-k relation near the top of the valence band and the bottom of the conduction band.



- The top of the valence band occurs at k=0 in most semiconductors.
- Notice the presence of two different E-k curves near the valence band edge, labelled the Heavy Hole and Light Hole bands.
- The bottom of the conduction band in some semiconductors occurs at k=0. Such semiconductors are called direct bandgap semiconductors. Examples include, GaAs and InP
- If the bottom of the conduction band does not occur at k=0, the semiconductor is termed indirect. Examples include Si and Ge.
- The alignment of the valence and conduction bandedges has important consequences. Direct bandgap semiconductors have a strong interaction with light. This is a result of the law of momentum conservation.

 When the conduction bandedge is at k=0, the band structure can be represented by:

$$E(k) = E_{C} + \frac{\hbar^{2}k^{2}}{2m^{*}}$$

- E_C is the conduction bandedge, and the band structure is a simple parabola.
- Notice that the E-k relation looks like that of an electron in free space except that the free electron mass m_0 is replaced by the effective mass m^* .
- The electron responds to the outside world as if it had this mass, of course the real electron mass does not change.
- The conduction band electron effective mass has a strong dependence on the bandgap, the smaller the bandgap the smaller the effective mass.

Indirect bandgap semiconductors

- In silicon the bottom of the conduction band occurs at six equivalent minima along the x, y and z-axis.
- The *k* values at the minima are:

 $\frac{2\pi}{a}(0.85,0,0), \frac{2\pi}{a}(0,0.85,0), \frac{2\pi}{a}(0,0.85)$

- And their inverses, where a (lattice constant) is 0.543nm for Si.
- For each of the six k points the conduction-band energy reaches a minimum value and as k moves away from these values the energy rises. These valleys in the conduction band have the energy momentum relationship:

$$\Xi(k) = E_{C} + \frac{\hbar^{2}}{2} \left[\frac{(k_{x} - k_{0x})^{2}}{m_{l}^{*}} + \frac{k_{y}^{2} + k_{z}^{2}}{m_{t}^{*}} \right]$$

- For valleys along the x-axis and -x-axis.
- m_{l}^{*} longitudinal effective mass $0.98m_{0}$. m_{t}^{*} transverse effective mass $0.19m_{0}$

Indirect bandgap semiconductors

What does this mean?

 The fact that the minimum in the conduction band does not occur at k=0 illustrates the main difference between particle momentum and crystal momentum.



- The particle momentum for a free electron is zero when the kinetic energy is zero.
- An electron at the conduction band minimum can have crystal momentum different from zero.
- In silicon when an electron makes a transition from the valence band to the conduction band, it requires not only an energy change but also a change in crystal momentum.

 The E-k relationships near the minimum of the conduction band or the maximum of the valence band are parabolic as indicated by:

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

• With a well known E-k relationship, the effective mass can be obtained from the second derivative of *E* with respect to hk: $\begin{bmatrix} d^2 E \end{bmatrix}^{-1}$

$$m^* = \left\lfloor \frac{d^2 E}{d(\hbar^2 k^2)} \right\rfloor$$

• Therefore the narrower the parabola, the smaller the effective mass. GaAs has a very narrow conduction band parabola and the electron effective mass is $0.07m_0$. For silicon it is $0.19m_0$ ([100]-direction).

Semiconductor DOS – Conduction Band

 Using effective mass instead of electron mass we can obtain a value for the density of states. Assuming an Ek relationship of the form:

$$\mathsf{E} = \mathsf{E}_{\mathsf{C}} + \frac{\hbar^2 \mathsf{k}^2}{2\mathsf{m}^*}$$

• The conduction band density of states becomes:

N(E) =
$$\frac{\sqrt{2}m^{*^{3/2}}(E - E_{C})^{1/2}}{\pi^{2}\hbar^{3}}$$
 : E ≥ E_C

- For indirect bandgap semiconductors, the conduction band density of states mass used in the above expression is: $m_{dos}^{*} = \left| 6^{2/3} (m_{l}^{*} m_{t}^{*2})^{1/3} \right|$
- For the valence band the density of states is: $N(E) = \frac{\sqrt{2}m *^{3/2} (E_v - E)^{1/2}}{\pi^2 \hbar^3} : E \le E_v$
- This is zero for $E > E_v$

• The energy-momentum relationship in the valence band is: $t^2 k^2 = t^2 k^2$

$$E = E_v - \frac{\hbar^2 k^2}{2m_{hh}^*}$$
 : $E = E_v - \frac{\hbar^2 k^2}{2m_{lh}^*}$

for the heavy hole and light hole bands respectively.

• The valence band density of states is hence:

$$N(E) = \frac{\sqrt{2}m_{hh}^{*3/2}(E_v - E)^{1/2}}{\pi^2 \hbar^3} + \frac{\sqrt{2}m_{lh}^{*3/2}(E_v - E)^{1/2}}{\pi^2 \hbar^3}$$
$$= \frac{\sqrt{2}m_{dos}^{*3/2}(E_v - E)^{1/2}}{\pi^2 \hbar^3}$$

 The density of states mass for the valence band is given by:

$$m_{dos}^{*3/2} = (m_{hh}^{*3/2} + m_{lh}^{*3/2})$$

• Calculate the k-value for an electron in the conduction band of GaAs with energy 0.1eV. Compare this to the case of an electron in free space.

$$\mathsf{k} = \frac{\sqrt{2\mathsf{m}\mathsf{E}}}{\hbar}$$

• For GaAs the appropriate mass in the conduction band is $0.067m_0$:

$$k = \frac{\left[2(0.067 \times 0.91 \times 10^{-30} \text{kg})(0.1 \times 1.6 \times 10^{-19} \text{J})\right]^{1/2}}{1.05 \times 10^{-34} \text{Js}}$$

$$= 4.2 \times 10^8 m^-$$

- In free space the value is: $k = 1.63 \times 10^9 m^{-1}$
- The two values are different since the k-value in the crystal represents the effective momentum.

Holes in semiconductors

- At finite temperatures electrons are promoted from the valence band to the conduction band. The valence band is left with unoccupied states.
- The concept of holes is introduced as a fictitious mathematic construction.
- It carries a positive charge and moves under the influence of an applied electric field, in a direction opposite to that of an electron.
- Mathematically, when all the valence band states are occupied, the sum over all wavevector states is zero:

$$\sum k_i = 0 = \sum_{k_i \neq k_e} k_i + k_e$$

• This says there are as many positive k states occupied as negative. In a situation where the electron at wavevector k_e is missing, the total wavevector is

$$\sum_{k_i \neq k_e} k_i = -k_e \text{ hole}$$

- As indicated previously. At finite temperatures electrons are promoted from the valence band to the conduction band.
- The combination of the electron and hole is termed an electron-hole pair. It is roughly the solid-state analogue of the ion pair in gases.
- The probability per unit time that an electron-hole pair is generated is given by:

$$p(T) = CT^{3/2} \exp\left(-\frac{E_g}{2k_BT}\right)$$

• T is the absolute temperature, E_g is the bandgap energy, k_B is the Boltzmann constant and C is a proportionality constant characteristic of the material.

- In the absence of an external electric field the created electron-hole pairs will recombine.
- An equilibrium is established in which the concentration of electron-hole pairs observed at any time is proportional to the rate of formation.
- This equilibrium concentration is a strong function of temperature and will decrease drastically if the material is cooled.

Band structure of Silicon

- Relatively easy to fabricate
- Excellent processing properties
- High-quality native oxide
- Bandgap is 1.1eV
- Has poor optical properties







Semiconductor Applications L2

- Germanium is an indirect semiconductor
- Bottom of conduction band occurs at 8 points.
- Hole properties of Ge are best of any semiconductor (low hole masses).
- Was the semiconductor of choice.
- Processesing considerations.
- Bandgap 0.9eV means that Ge must be cooled.
- Material of choice for gamma-ray based radiation detectors.



Properties of semiconductors

Property	Si	Ge	GaAs
Electron	m _l *=0.98		m*=0.067
effective mass	m _t *=0.19		
	m _{dos} *=1.08		
Hole	m _{hh} *=0.49		m _{hh} *=0.45
effective mass	m _{lh} *=0.16		m _{lh} *=0.08
	m _{dos} *=0.55		m _{dos} *=0.47
Bandgap (300K)	1.12eV	0.66eV	1.42eV
Bandgap (77K)	1.17eV	0.75eV	
Energy e-h pair (300K)	3.62eV		
Energy e-h pair (77K)	3.76eV	2.96eV	

A selection of important semiconductor properties

Properties of semiconductors

- At room temperature, the values of the bandgap are 1.12eV for silicon and 1.42eV for gallium arsenide.
- The bandgap approaches 1.17eV for Si and 1.52eV for GaAs at 0K.
- The variation with temperature can be expressed for Si: $(4.73 \times 10^{-4})T^{2}$

$$E_g(T) = 1.17 - \frac{(4.73 \times 10^{-1})T}{(T + 636)}$$

• For GaAs

$$E_g(T) = 1.52 - \frac{(5.4 \times 10^{-4})T^2}{(T + 204)}$$



- Calculate the effective momentum of an electron in the conduction band of GaAs when the electron energy measured from the bandedge is 0.5eV.
- E-k relation is $m^*=0.067m_0$:

$$\Xi - E_{\rm C} = \frac{\hbar^2 k^2}{2m^*}$$

• The effective momentum is hence:

$$\begin{split} \hbar k &= \sqrt{2m * (E - E_C)} \\ &= [2(0.067 \times 0.91 \times 10^{-30} \text{kg})(0.5 \times 1.6 \times 10^{-19} \text{J})]^{1/2} \\ &= 9.83 \times 10^{-26} \text{kgms}^{-1} \\ \text{k} &= 9.36 \times 10^8 \text{m}^{-1} \end{split}$$

• Free electron momentum

$$p = \sqrt{2m_0E} = 3.8 \times 10^{-25} kgms^{-1}$$

- Bandstructure in semiconductors:
 - Direct/indirect bandgaps
 - Density of states
 - Electrons and Holes
- E-k relationships for:
 - Silicon
 - GaAs
 - Germanium