PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 30: Chap. 13 of GGGPP

Basic properties of semiconductors

1. **Estimates of electron and hole concentrations in intrinsic semiconductors**
2. **Impurity states**

Lecture notes prepared using materials from GGGPP text.

22	Wed, 10/21/2015	Chap. 10	Scattering of particles by crystals	#20
23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
25	Wed, 10/28/2015	Chap. 11	Transport in metals	#23
26	Fri, 10/30/2015	Chap. 12	Optical properties of semiconductors and insulators	
27	Mon, 11/02/2015	Chap. 7 & 12	Excitons	#24
28	Wed, 11/04/2015	Chap. 9	Lattice vibrations	#25
29	Fri, 11/06/2015	Chap. 9	Lattice vibrations	#26
30	Mon, 11/09/2015	Chap. 13	Defects in semiconductors	#27
31	Wed, 11/11/2015	Chap. 14	Transport in semiconductors	
32	Fri, 11/13/2015	Chap. 14	Transport in semiconductors	
33	Mon, 11/16/2015	Chap. 15	Electron gas in Magnetic fields	
34	Wed, 11/18/2015	Chap. 17	Magnetic ordering in crystals	
35	Fri, 11/20/2015	Chap. 18	Superconductivity	
36	Mon, 11/23/2015	Chap. 18	Superconductivity	
	Wed, 11/25/2015		*Thanksgiving Holiday*	
	Fri, 11/27/2015		*Thanksgiving Holiday*	
37	Mon, 11/30/2015	Chap. 18	Superconductivity	
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	

Semiconductor properties

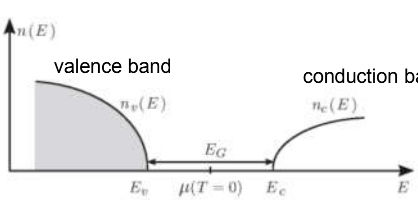


Figure 13.2 Schematic representation of the density-of-states of an intrinsic semiconductor. The top of the valence band is E_v and the bottom of the conduction band is E_c. The energy gap is $E_G = E_c - E_v$; the Fermi level at zero temperature lies at the middle of the band gap.

Boltzmann distribution for Fermi particles of energy *E*

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1},$$

chemical potential

Density of electrons in the conduction band at temperature *T*:

$$n_0(T) = \int_{E_c}^{\infty} n_c(E) f(E)\, dE = \int_{E_c}^{\infty} n_c(E) \frac{1}{e^{(E-\mu)/k_B T} + 1}\, dE.$$

Density of holes in the conduction band at temperature *T*:

$$p_0(T) = \int_{-\infty}^{E_v} n_v(E)(1 - f(E))\, dE = \int_{-\infty}^{E_v} n_v(E) \frac{1}{e^{(\mu-E)/k_B T} + 1}\, dE.$$

For an intrinsic semiconductor: $n_0(T) = p_0(T).$

Simplification of analysis for

$$E_c - \mu(T) \gg k_B T \quad \text{and} \quad \mu(T) - E_v \gg k_B T$$

$$n_0(T) = N_c(T) e^{-(E_c - \mu)/k_B T},$$

where

$$N_c(T) \equiv \int_{E_c}^{\infty} n_c(E) e^{-(E-E_c)/k_B T}\, dE.$$

$$p_0(T) = N_v(T) e^{-(\mu - E_v)/k_B T},$$

where

$$N_v(T) \equiv \int_{-\infty}^{E_v} n_v(E) e^{-(E_v - E)/k_B T}\, dE.$$

Chemical potential for intrinsic semiconductor

$$n_0(T) = p_0(T).$$

➔ $N_c(T) e^{-(E_c - \mu_i)/k_B T} = N_v(T) e^{-(\mu_i - E_v)/k_B T}.$

$$\boxed{\mu_i(T) = \frac{1}{2}(E_v + E_c) + \frac{1}{2} k_B T \ln \frac{N_v(T)}{N_c(T)}}$$

$$n_i(T) = p_i(T) = \sqrt{N_c(T) N_v(T)}\, e^{-E_G/2k_B T}.$$

Mass action relationship:

$$\boxed{n_0(T) p_0(T) = N_c(T) N_v(T) e^{-E_G/k_B T} \equiv n_i^2(T) = p_i^2(T)}.$$

Two parabolic band model

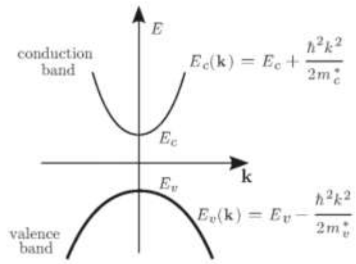


Figure 13.3 Isotropic two-band model semiconductor; the valence band profile has been reported in bold to remind its full occupancy by electrons at $T = 0$.

Two parabolic band model -- continued

$$n_c(E) = \int \frac{2}{(2\pi)^3} \delta(E_c(\mathbf{k}) - E)\, d\mathbf{k} = \int_0^\infty \frac{2}{(2\pi)^3} \delta\left(\frac{\hbar^2 k^2}{2m_c^*} + E_c - E\right) 4\pi k^2 dk.$$

$$n_c(E) = \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2}\right)^{3/2} (E - E_c)^{1/2} \quad \text{for} \quad E \geq E_c.$$

$$N_c(T) = \frac{\sqrt{\pi}}{2} \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2}\right)^{3/2} (k_B T)^{3/2}$$
$$= \frac{1}{4\pi^{3/2}} \left(\frac{m_c^*}{m} \frac{T}{T_0}\right)^{3/2} \left(\frac{k_B T_0}{\hbar^2/2ma_B^2}\right)^{3/2} \frac{1}{a_B^3}$$
$$= 2.534 \left(\frac{m_c^*}{m} \frac{T}{T_0}\right)^{3/2} \cdot 10^{19}\ \mathrm{cm}^{-3}.$$

For T_0=300 K

Two parabolic band model -- continued

Similar analysis of valence band:

$$N_v(T) = \frac{\sqrt{\pi}}{2} \frac{1}{2\pi^2} \left(\frac{2m_v^*}{\hbar^2}\right)^{3/2} (k_B T)^{3/2}.$$

Chemical potential

$$\mu_i(T) = \frac{1}{2}(E_v + E_c) + \frac{3}{4} k_B T \ln \frac{m_v^*}{m_c^*}.$$

Effects of impurities

Bloch states of perfect lattice

$$\left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right]\psi_n(\mathbf{k},\mathbf{r}) = E_n(\mathbf{k})\psi_n(\mathbf{k},\mathbf{r});$$

Schroedinger equation for system with impurities

$$\left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + V_I(\mathbf{r})\right]\phi(\mathbf{r}) = E\phi(\mathbf{r}).$$

Expression of impurity wavefunction in terms of Bloch states:

$$\phi(\mathbf{r}) = \sum_{n'\mathbf{k}'} A_{n'}(\mathbf{k}')\psi_{n'}(\mathbf{k}',\mathbf{r}).$$

Effects of impurities -- continued

$$\phi(\mathbf{r}) = \sum_{n'\mathbf{k}'} A_{n'}(\mathbf{k}')\psi_{n'}(\mathbf{k}',\mathbf{r}).$$

$$[E_n(\mathbf{k}) - E]A_n(\mathbf{k}) + \sum_{n'\mathbf{k}'} U_{nn'}(\mathbf{k},\mathbf{k}')A_{n'}(\mathbf{k}') = 0,$$

where $U_{nn'}(\mathbf{k},\mathbf{k}') = \int \psi_n^*(\mathbf{k},\mathbf{r})V_I(\mathbf{r})\psi_{n'}(\mathbf{k}',\mathbf{r})\,d\mathbf{r}.$

For two parabolic band model

Case for impurity states near conduction band

$$\left[\frac{\hbar^2k^2}{2m_c^*} + E_c - E\right]A(\mathbf{k}) + \sum_{\mathbf{k}'} U(\mathbf{k},\mathbf{k}')A(\mathbf{k}') = 0,$$

$$U(\mathbf{k},\mathbf{k}') = \int \psi_c^*(\mathbf{k},\mathbf{r})V_I(\mathbf{r})\psi_c(\mathbf{k}',\mathbf{r})\,d\mathbf{r}.$$

Case for impurity states near conduction band -- continued

$$U(\mathbf{k},\mathbf{k}') = \int u_c^*(\mathbf{k},\mathbf{r})u_c(\mathbf{k}',\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}V_I(\mathbf{r})\,d\mathbf{r}.$$

$$\approx \frac{1}{V}\int e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}V_I(\mathbf{r})\,d\mathbf{r};$$

Define envelope function $F(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} A(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}},$

$$\left[-\frac{\hbar^2}{2m_c^*}\nabla^2 + V_I(\mathbf{r})\right]F(\mathbf{r}) = (E - E_c)F(\mathbf{r}).$$

Case for impurity states near conduction band -- continued

$$\left[-\frac{\hbar^2}{2m_c^*}\nabla^2 - \frac{e^2}{\varepsilon_s r}\right]F(\mathbf{r}) = (E-E_c)F(\mathbf{r}).$$

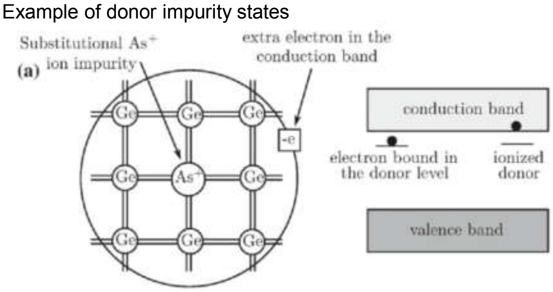
approximation to V_I

Bound states – donor levels

$$\varepsilon_d = E_c - E_d = 13.606\frac{m_c^*}{m}\frac{1}{\varepsilon_s^2}\ (\text{eV}).$$

$$a_d = a_B\frac{m}{m_c^*}\varepsilon_s.$$

Example of donor impurity states



Case for impurity states near valence band

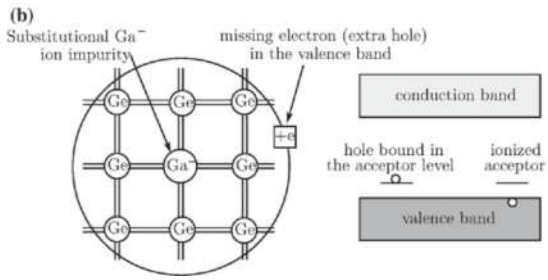
$$\left[+\frac{\hbar^2}{2m_v^*}\nabla^2 + V_I(\mathbf{r})\right]F(\mathbf{r}) = (E-E_v)F(\mathbf{r}).$$

$$\left[-\frac{\hbar^2}{2m_v^*}\nabla^2 - \frac{e^2}{\varepsilon_s r}\right]F(\mathbf{r}) = -(E-E_v)F(\mathbf{r}).$$

Bound state solutions for accepter impurity levels

$$\varepsilon_a = E_a - E_v = 13.606\frac{m_v^*}{m}\frac{1}{\varepsilon_s^2}\ (\text{eV}).$$

Example of acceptor impurity states



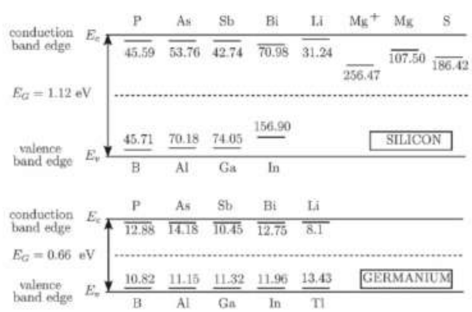


Figure 13.5 Experimental ionization energies (meV) for various donor and acceptor impurities (upper and lower part of the panels, respectively) in silicon and germanium. For donor impurities, the electron binding energy $\varepsilon_d = E_c - E_d$ is reported; for acceptor impurities the hole binding energy $\varepsilon_a = E_a - E_v$ is reported. The data are taken from A. K. Ramdas and S. Rodriguez, Rep. Progr. Phys. *44*, 1297 (1981).

Mobile electrons and holes in doped semiconductors as a function of temperature

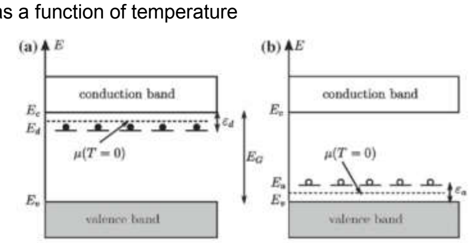


Figure 13.7 (a) Schematic representation of the energy levels of a homogeneously doped n-type semiconductor at $T = 0$ (in abscissa any arbitrary direction in the homogeneous material can be considered). Typical energy values are $E_G = E_c - E_v \approx 1$ eV and $\varepsilon_d = E_c - E_d \approx 10$ meV. The Fermi level at zero temperature lies at $(1/2)(E_d + E_c)$, which is the middle point between E_d and E_c. (b) Schematic representation of the energy levels of a homogeneously doped p-type semiconductor at $T = 0$; typical values of $\varepsilon_a = E_a - E_v$ are of the order of 10 meV. The Fermi level at zero temperature lies at $(1/2)(E_v + E_a)$, which is the middle point between E_v and E_a.

Probability that E_d is occupied by an electron of either spin

$$P(E_d) = \frac{1}{(1/2)e^{(E_d-\mu)/k_BT} + 1};$$

Density of electrons in conduction band

$$\boxed{n_0(T) = N_d[1 - P(E_d)] + p_0(T)},$$

$$N_c(T)e^{-(E_c-\mu)/k_BT} = N_d \frac{(1/2)e^{(E_d-\mu)/k_BT}}{(1/2)e^{(E_d-\mu)/k_BT} + 1} + N_v(T)e^{-(\mu-E_v)/k_BT}.$$

At low temperature: $N_c(T)e^{-(E_c-\mu)/k_BT} = \frac{1}{2}N_d\, e^{(E_d-\mu)/k_BT};$

$$n_0(T) = N_c(T)e^{-(E_c-\mu)/k_BT} = \sqrt{N_c(T)\frac{N_d}{2}}\, e^{-\varepsilon_d/2k_BT}.$$

At moderate temperatures

$$n_0(T) = N_c(T)e^{-(E_c-\mu)/k_BT} \cong N_d;$$

$$\mu(T) = E_c + k_BT \ln \frac{N_d}{N_c(T)}.$$

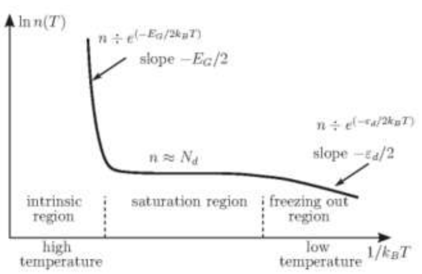


Figure 13.8 Schematic variation of the electron concentration as a function of $1/k_BT$ in an n-type semiconductor with N_d donor impurities per unit volume.

Note that similar analysis applies to the acceptor levels; in general a given semiconductor can have concentrations of both N_d donors and N_a acceptors.