PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

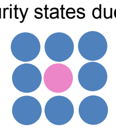
Plan for Lecture 25:

- Chap. 18 & 19 in Marder
  - Impurity states
  - Properties of semiconductors

Some of the lecture materials are from slides prepared by Marder

21	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015
24	Wed: 03/25/2015	Chap. 17 & 18	Electron Transport		
25	Fri: 03/27/2015	Chap. 18	Microscopic picture of transport	#23	03/30/2015
26	Mon: 03/30/2015				04/01/2015
27	Wed: 04/01/2015				04/06/2015
	Fri: 04/03/2015	Good Friday	No class		
28	Mon: 04/06/2015				04/08/2015
29	Wed: 04/08/2015				04/10/2015
30	Fri: 04/10/2015				04/13/2015
31	Mon: 04/13/2015				04/15/2015
32	Wed: 04/15/2015				04/17/2015
33	Fri: 04/17/2015				04/20/2015
34	Mon: 04/20/2015				
35	Wed: 04/22/2015				
36	Fri: 04/24/2015				
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

Impurity states due to point defects



$$(H_0 + V)\Psi = E\Psi$$

Unperturbed Hamiltonian: $H_0\phi_{n\mathbf{k}} = \epsilon_{n\mathbf{k}}\phi_{n\mathbf{k}}$

Expand Ψ as a superposition of Bloch waves:

$$\Psi = \sum_{n\mathbf{k}} C_{n\mathbf{k}}\phi_{n\mathbf{k}}$$

Equation for expansion coefficients:

$$\epsilon_{n\mathbf{k}}C_{n\mathbf{k}} + \sum_{n'\mathbf{k}'}\langle n\mathbf{k}|V|n'\mathbf{k}'\rangle C_{n'\mathbf{k}'} = EC_{n\mathbf{k}}$$

Impurity states due to point defects -- continued

Define:

$$F_n(\mathbf{r}) \approx \sum_{\mathbf{k}} C_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\Psi(\mathbf{r}) \approx \sum_{\mathbf{k}} \phi_{n\mathbf{k}}(\mathbf{r}) \int d^3s F_n(\mathbf{s}) e^{-i\mathbf{k}\cdot\mathbf{s}}$$

Suppose that for impurity states near the conduction band edge: $\epsilon_{n\mathbf{k}} = \epsilon_c + \frac{\hbar^2 k^2}{2m_c^*}$

Suppose that for impurity states near the valence band edge: $\epsilon_{n\mathbf{k}} = \epsilon_v - \frac{\hbar^2 k^2}{2|m_v^*|}$

Impurity states due to point defects -- continued

$$V(\mathbf{r}) \approx -\frac{Z_{eff} e^2}{\epsilon r}$$

Z_{eff}: valence charge of impurity relative to that of host lattice

ϵ: Dielectric constant

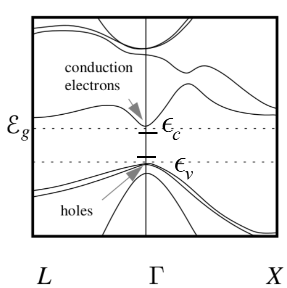
Equation for wavepacket amplitudes

$$\epsilon_{n\mathbf{k}} = \epsilon_c + \frac{\hbar^2 k^2}{2m_c^*} \approx \epsilon_c - \frac{\hbar^2 \nabla^2}{2m_c^*} \qquad \left(\epsilon_c - \frac{\hbar^2 \nabla^2}{2m_c^*} - \frac{Z_{eff} e^2}{\epsilon r}\right) F(\mathbf{r}) = EF(\mathbf{r})$$

$$\epsilon_{n\mathbf{k}} = \epsilon_v - \frac{\hbar^2 k^2}{2|m_v^*|} \approx \epsilon_v + \frac{\hbar^2 \nabla^2}{2|m_v^*|} \qquad \left(\epsilon_v + \frac{\hbar^2 \nabla^2}{2|m_v^*|} + \frac{|Z_{eff}| e^2}{\epsilon r}\right) F(\mathbf{r}) = EF(\mathbf{r})$$

Impurity states due to point defects -- continued

Gallium arsenide



Electron impurity:

$$E = \epsilon_c - \frac{m_c^* Z_{eff}^2 e^4}{2\epsilon^2 \hbar^2 n^2}$$

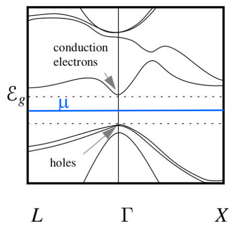
Hole impurity:

$$E = \epsilon_v + \frac{|m_v^*| Z_{eff}^2 e^4}{2\epsilon^2 \hbar^2 n^2}$$

Semiconductor properties

Population of electrons (n) and holes (p) in a pure semiconductor

Gallium arsenide



$$n = \int_{\mathcal{E}_c}^{\infty} d\mathcal{E}\, D(\mathcal{E}) \frac{1}{e^{\beta(\mathcal{E}-\mu)}+1},$$

$$p = \int_{-\infty}^{\mathcal{E}_v} d\mathcal{E}\, D(\mathcal{E}) \left\{1 - \frac{1}{e^{\beta(\mathcal{E}-\mu)}+1}\right\}$$

Semiconductor properties -- continued

For: $\mathcal{E}_c - \mu \gg k_B T$ and $\mu - \mathcal{E}_v \gg k_B T.$

$$n = \mathcal{N}_c e^{-\beta(\mathcal{E}_c - \mu)}, \quad p = \mathcal{N}_v e^{-\beta(\mu - \mathcal{E}_v)}$$

$$\mathcal{N}_c = \int_{\mathcal{E}_c}^{\infty} d\mathcal{E}\, D(\mathcal{E}) e^{-\beta(\mathcal{E}-\mathcal{E}_c)}$$

$$\mathcal{N}_v = \int_{-\infty}^{\mathcal{E}_v} d\mathcal{E}\, D(\mathcal{E}) e^{-\beta(\mathcal{E}_v-\mathcal{E})}.$$

Semiconductor properties -- continued

$$D(\mathcal{E}) = 2\int m_n^{\star 3/2} \frac{d\vec{q}}{(2\pi)^3} \delta\left(\mathcal{E} - \mathcal{E}_c - \frac{1}{2}\hbar^2 q^2\right)$$

$$= \sqrt{2(\mathcal{E}-\mathcal{E}_c)} \frac{m_n^{\star 3/2}}{\hbar^3 \pi^2} \mathcal{M}_c$$

multiplicity of conduction band minima

$$\mathcal{N}_c = \frac{1}{4}\left(\frac{2 m_n^{\star} k_B T}{\pi \hbar^2}\right)^{3/2} \mathcal{M}_c$$

$$\mathcal{N}_v = \frac{1}{4}\left(\frac{2 m_p^{\star} k_B T}{\pi \hbar^2}\right)^{3/2}.$$

Semiconductor properties -- continued

$$n = \mathcal{N}_c e^{-\beta(\mathcal{E}_c - \mu)}, \quad p = \mathcal{N}_v e^{-\beta(\mu - \mathcal{E}_v)}$$

$$np = \mathcal{N}_c \mathcal{N}_v e^{-\beta \mathcal{E}_g}.$$

For intrinsic semiconductor, $n=p=n_i$

$$n_i = \sqrt{\mathcal{N}_c \mathcal{N}_v} e^{-\beta \mathcal{E}_g/2}$$

$$\mu_i = k_B T \ln \frac{n_i}{\mathcal{N}_c} + \mathcal{E}_c = \mathcal{E}_v + \frac{\mathcal{E}_g}{2} + \frac{3}{4} k_B T \ln(m_p^\star / m_n^\star) - \frac{1}{2} k_B T \ln \mathcal{M}_c.$$

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Semiconductor properties -- continued

Intrinsic carriers: $np = n_i^2$

$$n = n_i e^{-\beta(\mu_i - \mu)}, \quad p = n_i e^{-\beta(\mu - \mu_i)}.$$

Effects of impurities:

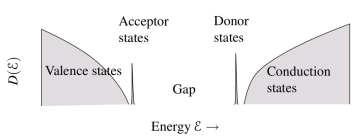

Figure 19.10: Densities of states with doping

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Semiconductor properties – continued

Typically, the ionized impurities dominate the carrier concentrations

$$n - p = \mathcal{N}_d - \mathcal{N}_a.$$

$$n = \frac{1}{2}[\mathcal{N}_d - \mathcal{N}_a] + \frac{1}{2}\left[(\mathcal{N}_d - \mathcal{N}_a)^2 + 4n_i^2\right]^{1/2}$$

$$p = \frac{1}{2}[\mathcal{N}_a - \mathcal{N}_d] + \frac{1}{2}\left[(\mathcal{N}_d - \mathcal{N}_a)^2 + 4n_i^2\right]^{1/2}.$$

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Semiconductor properties – continued

$$n - p = 2n_i \sinh \beta(\mu - \mu_i)$$
$$\mu = \mu_i + k_B T \sinh^{-1}\left([\mathcal{N}_d - \mathcal{N}_a]/2n_i\right).$$

For primarily donor doping:

$$n \approx \mathcal{N}_d$$
$$p \approx \frac{n_i^2}{\mathcal{N}_d}.$$

For primarily acceptor doping:

$$p \approx \mathcal{N}_a$$
$$n \approx \frac{n_i^2}{\mathcal{N}_a}.$$

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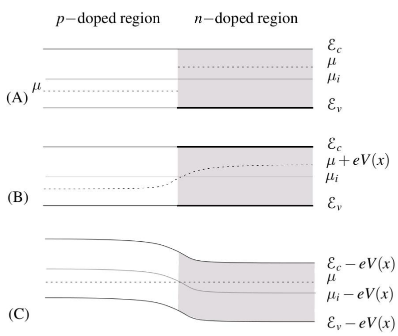
Semiconductor junction



Before equilibration

After equilibration

Junction potential

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Semiconductor junction

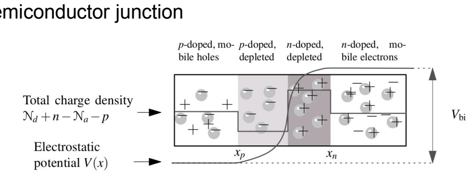

Figure 19.15: Illustration of the redistribution of mobile charges near a p–n junction.

$$n(x) = n_i e^{\beta(\mu + eV(x) - \mu_i)}$$
$$p(x) = n_i e^{\beta(\mu_i - eV(x) - \mu)}.$$

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Semiconductor junction

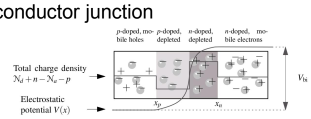


Figure 19.15: Illustration of the redistribution of mobile charges near a p–n junction.

$$en_{\text{ions}} = e[\mathcal{N}_d(x) - \mathcal{N}_a(x)].$$

$$\frac{\partial^2 V}{\partial x^2} = -4\pi e[\mathcal{N}_d(x) - n(x) - \mathcal{N}_a(x) + p(x)]/\epsilon^0,$$

Semiconductor junction

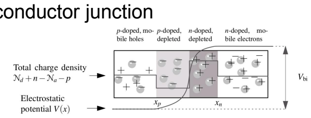


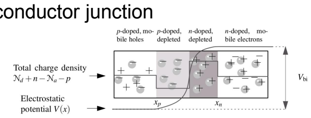
Figure 19.15: Illustration of the redistribution of mobile charges near a p–n junction.

Simplified model:

$$\begin{aligned} \mathcal{N}_a(x) &= \mathcal{N}_a\theta(-x) \\ \mathcal{N}_d(x) &= \mathcal{N}_d\theta(x). \end{aligned}$$

$$V(x) = \begin{cases} V(-\infty) & \text{for } x < x_p \\ V(-\infty) + 2\pi e\frac{\mathcal{N}_a}{\epsilon^0}(x-x_p)^2 & \text{for } 0 > x > x_p \\ V(\infty) \quad - 2\pi e\frac{\mathcal{N}_d}{\epsilon^0}(x-x_n)^2 & \text{for } 0 < x < x_n \\ V(\infty) & \text{for } x > x_n. \end{cases}$$

Semiconductor junction



$$\begin{aligned} n(\infty)p(-\infty) &= \mathcal{N}_d\mathcal{N}_a = n_i^2 e^{\beta(eV(\infty)-eV(-\infty))} \\ \Rightarrow eV_{\text{bi}} &\equiv e[V(\infty) - V(-\infty)] \\ &= k_BT\ln\frac{\mathcal{N}_d\mathcal{N}_a}{n_i^2} = \mathcal{E}_g + k_BT\ln[\frac{\mathcal{N}_d\mathcal{N}_a}{\mathcal{N}_c\mathcal{N}_v}], \end{aligned}$$

$$V(-\infty) + 2\pi e\frac{\mathcal{N}_a}{\epsilon^0}x_p^2 = V(\infty) - 2\pi e\frac{\mathcal{N}_d}{\epsilon^0}x_n^2,$$

$$\mathcal{N}_d x_n = -\mathcal{N}_a x_p.$$

$$\begin{aligned} x_n &= \sqrt{\frac{\epsilon^0\mathcal{N}_a V_{\text{bi}}}{2\pi e\mathcal{N}_d[\mathcal{N}_a+\mathcal{N}_d]}} \\ x_p &= -\sqrt{\frac{\epsilon^0\mathcal{N}_d V_{\text{bi}}}{2\pi e\mathcal{N}_a[\mathcal{N}_a+\mathcal{N}_d]}}, \end{aligned}$$

Behavior of ideal diode

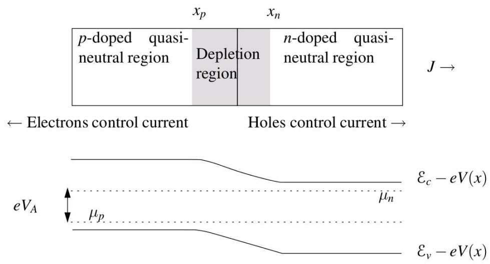


Figure 19.16: Sketch of p–n junction in forward bias

Behavior of ideal diode – continued

Diffusion of electrons and holes:

$$j_n = e\mathcal{D}_n \vec{n}' \qquad \text{where: } n' \equiv \nabla n$$
$$j_p = -e\mathcal{D}_p \vec{p}' \qquad p' \equiv \nabla p$$

$$n(x) = \mathcal{N}_d e^{\beta e[V(x)-V(x_n)]}\left[1 + \frac{j_n}{e\mathcal{N}_d \mathcal{D}_n}\int_{x_n}^{x} dx'\, e^{-\beta e[V(x')-V(x_n)]}\right]$$
$$p(x) = \mathcal{N}_a e^{-\beta e[V(x)-V(x_p)]}\left[1 - \frac{j_p}{e\mathcal{N}_a \mathcal{D}_p}\int_{x_p}^{x} dx'\, e^{\beta e[V(x')-V(x_p)]}\right]$$