6.730 Physics for Solid State Applications

Lecture 26: Inhomogeneous Solids

Outline

- Electrochemical Potential
- Inhomogeneous Solids in Equilibrium
- PN Junctions

April 9, 2004

Electrochemical potential

The electrochemical potential, a.k.a, the fermi level is $\mu = \left(\frac{\partial E}{\partial N}\right)_S$

The energy can be divided into two parts if the particle has charge

$$E = E_{\text{orbital,nocharge}} + E_{\text{electrostatic,withcharge}}$$

$$\Rightarrow \quad \mu = \left(\frac{\partial E_{\text{orbital}}}{\partial N}\right)_S + \left(\frac{\partial E_{\text{electrostatic}}}{\partial N}\right)_S$$

If the electric field is $\mathbf{E}(r) = -\nabla\phi$

then the change in electrostatic energyis $dE = -e\,\phi\,dN$

$$\Rightarrow \quad \mu = \mu' - e\,\phi(x)$$

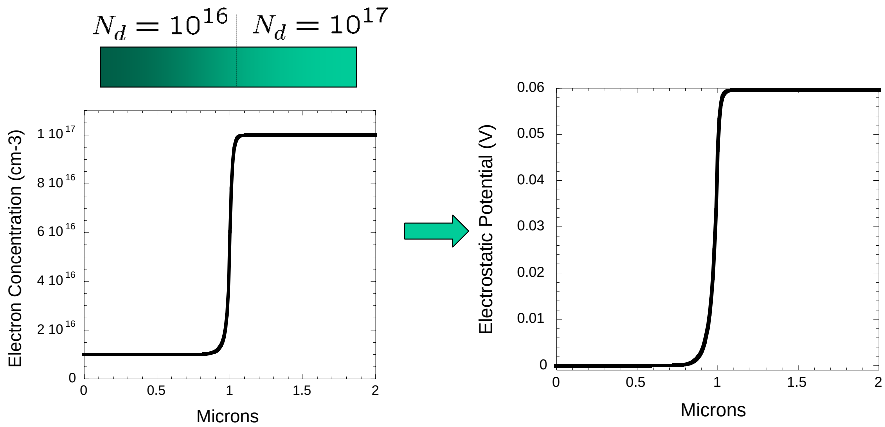
Fermi level or the electrochemical potential (μ)

the electrochemical potential for an electrically neutral particle (μ')

Inhomogeneous Semiconductors in Equilibrium

Inhomogeneous doping

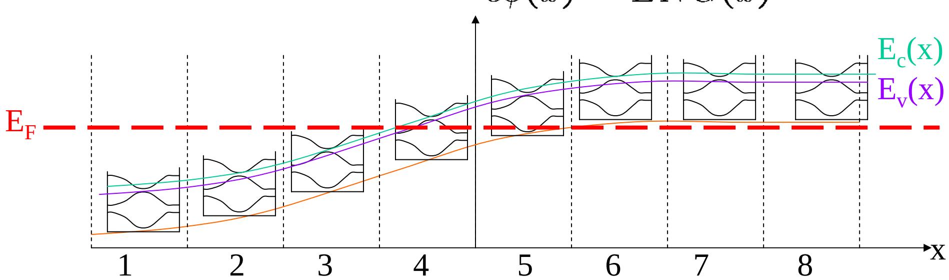
Consider a solid with a spatially varying impurity concentration...



In equilibrium, the carrier concentration is balanced by an internal electrostatic potential...why?

Slowly varying potentials

$$-e\phi(x) = ENG(x)$$



1. Break up the material into regions where $\phi(x)$ is nearly constant
2. Assume Range of $\phi(x)$ >> range of wavepacket >> lattice constant
3. Each region has the same electrochemical potential (equilibrium) so that $\mu = \mu_i' - e\,\phi_i$ is the same for each region.
4. Each characteristic energy of the energy bands changes with position
5. The electrochemical potential $E_F = \mu$ is independent of position!

Inhomogeneous Semiconductors in Equilibrium

If electrostatic potential varies slowly compared to wavepacket...

$$\left(-\frac{\hbar^2\nabla^2}{2m^*} + E_{co} - q\phi(r)\right) F(r) = EF(r)$$

Dividing solid into slices where ϕ_i is uniform and depends only on x...

$$-\frac{\hbar^2\nabla^2}{2m^*} F_i(r) = (E_i - E_{co} + q\phi_i)\, F_i(r)$$

...the envelope function has solutions of the form...

$$F_i(r) = \left(A_i e^{ik_x x} + B_i e^{-ik_x x}\right) e^{+ik_y y} e^{+ik_z z}$$

...therefore the eigenenergies are...

$$E_i = E_{co} - q\phi_i + \frac{\hbar^2 k^2}{2m^*} \quad \Rightarrow \quad E(r) = E_{co} - q\phi(x) + \frac{\hbar^2 k^2}{2m^*}$$

Inhomogeneous Semiconductors in Equilibrium

Given the modified energy levels, the 3-D DOS becomes....

$$g(E,r) = \frac{1}{2\pi^2\hbar^3}(2m^*)^{3/2}\left[E - E_{co} + q\phi(r)\right]^{1/2}$$

...in equilibrium the carrier concentration is with $\mu = E_F$...

$$n(r) = \int_{E_{co}-q\phi(r)}^{\infty} g(E,r)\frac{1}{1+e^{(E-E_F)/k_BT}}dE$$

$$= \frac{2}{\sqrt{\pi}} N_c\, F_{1/2}\left(\frac{E_F - E_{co} + q\phi(r)}{k_BT}\right)$$

$$\approx N_c \exp\left(\frac{-(E_{co} - q\phi(r) - E_F)}{k_BT}\right)$$ Boltzmann approx.

Inhomogeneous Semiconductors in Equilibrium

$$n(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_{co} + q\phi(r)}{k_B T}\right)$$

$$E_c(r) \equiv E_{co} - q\phi(r)$$

$$n(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_c(r)}{k_B T}\right)$$

$$\approx N_c \exp\left(\frac{-(E_c(r) - E_F)}{k_B T}\right)$$

The electrostatic potential is incorporated in $E_c(r)$ or $E_v(r)$

$$p(r) = \frac{2}{\sqrt{\pi}} N_v F_{1/2}\left(\frac{E_v(r) - E_F}{k_B T}\right) \approx N_c \exp\left(\frac{-(E_F - E_v(r))}{k_B T}\right)$$

Inhomogeneous Semiconductors in Equilibrium

$$E_c(r) \equiv E_{co} - q\phi(r)$$

Density with field

$$n(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_c(r)}{k_B T}\right) \approx N_c \exp\left(\frac{-(E_c(r) - E_F)}{k_B T}\right)$$

Background Density without field

$$n_o = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_c}{k_B T}\right) \approx N_c \exp\left(\frac{-(E_c - E_F)}{k_B T}\right)$$

The potential satisfies Poisson's Equation

$$\frac{\partial^2}{\partial x^2}\phi(x) = -\frac{e}{\epsilon}\left[n_o(r) - n_o\right]$$

With boundary conditions at the interface,

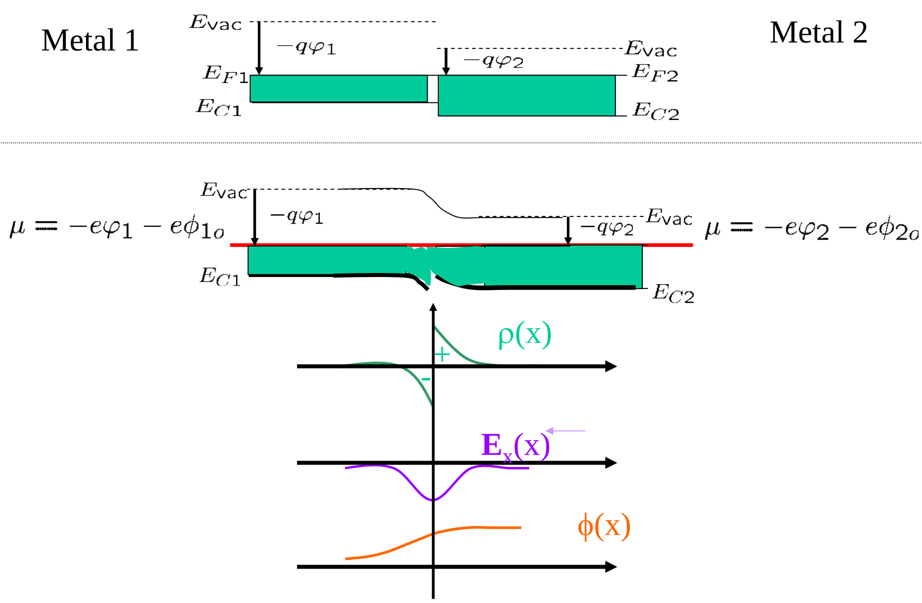
$$-\epsilon_1 \frac{\partial}{\partial x}\phi_1(x) + \epsilon_2 \frac{\partial}{\partial x}\phi_2(x) = Q_{interface}$$

Example: Metal-Metal contact

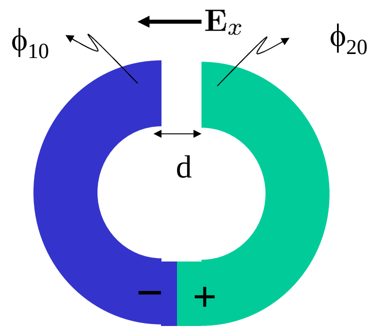
E_{vac} is a reference level: In the absence of image forces, this is the energy needed to remove an electron from EF so that the material no longer influences it.

When the metals are brought together so that electrons can tunnel from one to the other, particles will be exchanged until $\bar{\mu}$ is the same.

Metal-Metal contact



electrochemical potentials and work functions



$\varphi_1 > \varphi_2$

The electric field in the gap $\mathbf{E}_x = -\frac{\phi_{20} - \phi_{10}}{d}$

Recall that $\mu = -e\varphi_1 - e\phi_{10} = -e\varphi_2 - e\phi_{20}$

$$\mathbf{E}_x = -\frac{\varphi_1 - \varphi_2}{d}$$ which is the negative x direction

Self-consistent potential: metals and semiconductors

$$n(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_c(r)}{k_B T}\right)$$

Density with field

$$n_o = \frac{2}{\sqrt{\pi}} N_c F_{1/2}\left(\frac{E_F - E_c}{k_B T}\right)$$

Background Density without field

The potential satisfies Poisson's Equation $\frac{\partial^2}{\partial x^2}\phi(x) = -\frac{e}{\epsilon}\left[n(r) - n_o\right]$

With boundary conditions, $-\epsilon_1 \frac{\partial}{\partial x}\phi_1(x) + \epsilon_2 \frac{\partial}{\partial x}\phi_2(x) = Q_{interface}$

$$\frac{\partial^2}{\partial x^2}\phi(x) = -\frac{e}{\epsilon}\left[n(r) - n_o\right]$$

$$\approx -\frac{e}{\epsilon}\frac{\partial}{\partial E_F} n(r)|_{\phi=0}(-e\phi(x))$$

$$\approx \frac{1}{L_i^2}\phi(x)$$ where the Debye length is $L_i = \sqrt{\frac{\epsilon}{e^2 \frac{\partial}{\partial E_F} n}}$

Debye Lengths

$$\frac{\partial^2}{\partial x^2}\phi(x) \approx \frac{1}{L_i^2}\phi(x)$$

where the Debye length is $L_i = \sqrt{\dfrac{\epsilon}{e^2 \frac{\partial}{\partial E_F} n}}$

$\frac{\partial}{\partial E_F} n = g(E_F)$ for a metal, and L is a fraction of an Angstrom

$\frac{\partial}{\partial E_F} n = \frac{n}{k_B T}$ for a semicondutor, and L is a few microns

Potential profile

$$\frac{\partial^2}{\partial x^2}\phi(x) \approx \frac{1}{L_i^2}\phi(x)$$

The solution for the potential is:

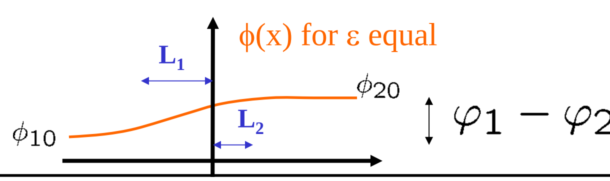
$$\phi_1(x) = \phi_{10} + A_1\, e^{x/L_1} \quad \text{for } x < 0$$

$$\phi_2(x) = \phi_{20} + A_2\, e^{-x/L_2} \quad \text{for } x > 0$$

with the boundary condition of no surface charge, one finds

$$\phi_1(x) = \phi_{10} + \frac{L_1/\epsilon_1}{L_1/\epsilon_1 + L_2/\epsilon_2}(\varphi_1 - \varphi_2)\, e^{x/L_1} \quad \text{for } x < 0$$

$$\phi_2(x) = \phi_{20} - \frac{L_2/\epsilon_2}{L_1/\epsilon_1 + L_2/\epsilon_2}(\varphi_1 - \varphi_2)\, e^{-x/L_2} \quad \text{for } x > 0$$



Example: PN-junction