Answers to Exam - Solid State Physics

Wednesday, 2nd November 2016, $09:00 - 12:00$

This is a closed-book exam. You are not allowed to bring books, notes etc. You can use a basic or scientific calculator, but no other electronic equipment with capabilities to display or pronounce the course content.

Do not forget to indicate your full name and student number on __each__ sheet. Please write in a clear way!

There are 5 problems with total points of 100.

1) **Crystal structure (15 points).**

   a. In graphene carbon atoms form a honeycomb lattice as shown in figure 1, however it is not a Bravais lattice. Find the corresponding Bravais lattice for graphene. Draw the basis and primitive lattice vectors. **(8 pt.)**
   b. Structure of graphite can be considered as graphene layers stacked together, as shown in figure 2. What is corresponding Bravais lattice? Give your argument. **(4 pt.)**
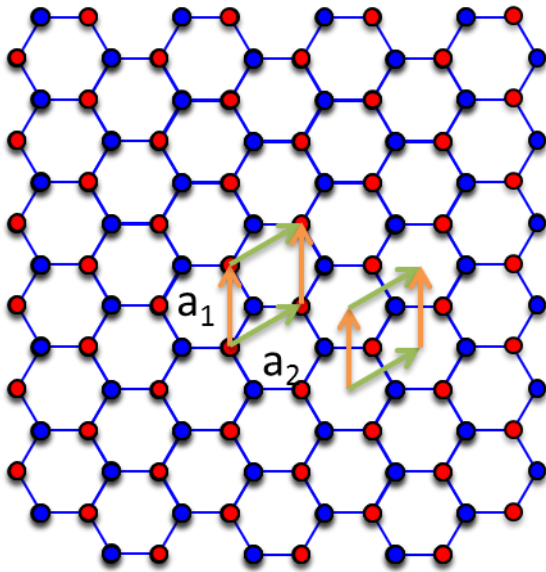   **c.** How many carbon atoms are there in the primitive cell of graphite? **(3 pt.)**
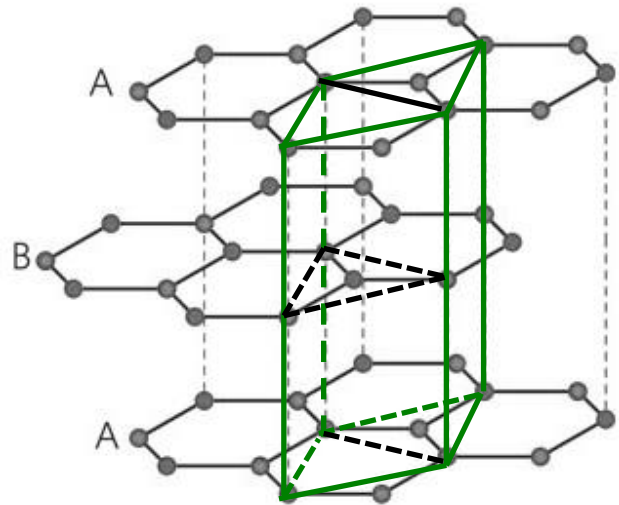
Figure 1

Figure 2

a. Primitive lattice vectors are a_1 and a_2 respectively. Basis consists of two carbon atoms (*sublattice A* and *sublattice B* denoted by *red* and *blue* colors). Each sublattice forms hexagonal lattice. Bravais lattice for graphene is hexagonal lattice.

b. Hexagonal (NOT HCP, since the atom in the middle of the hexagonal structure is missing).

c. The unit cell of graphite can be chosen as in the picture. In the upper or lower layer we have $\frac{1}{2}\left(1 + 2 \cdot \frac{1}{6} + 2 \cdot \frac{1}{3}\right) = 1$ atom. In the middle plane we have

$$\left(1 + 2 \cdot \frac{1}{6} + 2 \cdot \frac{1}{3}\right) = 2 \text{ atoms so in total 4 atoms.}$$

2) X-Ray diffraction in crystals (20 points).

There exist hollow molecules entirely made of carbon atoms, the most famous one is C_{60}, a molecule made of 60 carbon atoms arranged in the form of a icosahedron: that is, C_{60} has roughly the shape of a sphere. C_{60} molecules crystallize in an **FCC** lattice of charge-neutral molecules with cubic lattice constant $a = 14.11$ Å.

a. What kind of cohesive forces keep the molecules together in this crystal? **(2 pt.)**

b. We know from experiment that in a C_{60} molecule the distance from the carbon nuclei to the center of the molecule is $R = 3.5$ Å. Assume that 360 electrons are uniformly distributed on the surface of C_{60} molecule, such that the electron density can be written as $n(\mathbf{r}) = A\,\delta(|\mathbf{r}| - R)$, where the δ is a delta function. Determine the constant A. **(5 pt.)**

c. Determine the *atomic form factor* f_G as a function of the reciprocal lattice vector G. **(5 pt.)**

d. Calculate the *Structure Factor* for the $(2\,0\,0)$ and $(1\,1\,1)$ planes. Explain from your result why, experimentally, the $(2\,0\,0)$ X-ray diffraction peak is much weaker (~5%) compared to the $(1\,1\,1)$ peak. **(8 pt.)**

Hint: Structure factor for **FCC** lattice is

$$S_G = f_G\left(1 + e^{-i\pi(h+k)} + e^{-i\pi(k+l)} + e^{-i\pi(h+l)}\right)$$

Atomic form factor is

$$f_G = 4\pi \int\limits_0^\infty dr \cdot n(r) \cdot r^2 \cdot \frac{sin(\mathbf{G}\cdot\mathbf{r})}{\mathbf{G}\cdot\mathbf{r}}$$
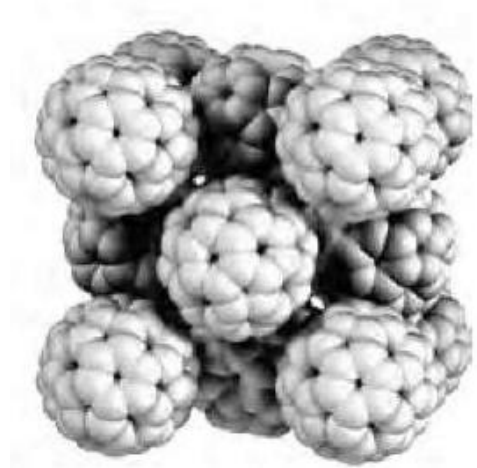
Solution

a. The lattice consists of neutral atoms, so there are no ionic bonds between atoms, neither covalent bonds. The cohesive force is van der Waals force.

b. There are 360 electrons spread over an area of the shell $4\pi R^2 = 154\,\text{Å}^2$. This gives a density of $A = 2.34$ electrons Å^{-2},

$n(R) = \frac{N}{4\pi R^2}$, so $A = \frac{360}{4\pi(3.5A)^2} \approx 2.3\,\text{Å}^{-2}$, or using the electron charge,

$A = 3.7\ x\ 10^{-19}\,C\,\text{Å}^{-2}$.

c.

$$f_j = 4\pi \int dr \cdot n(r) \cdot r^2 \cdot \frac{sin(\boldsymbol{G} \cdot \boldsymbol{r})}{\boldsymbol{G} \cdot \boldsymbol{r}} = A \cdot 4\pi \int dr \cdot \delta(|\boldsymbol{r}| - R) \cdot r^2 \cdot \frac{sin(\boldsymbol{G} \cdot \boldsymbol{r})}{\boldsymbol{G} \cdot \boldsymbol{r}}$$

$$= A \cdot 4\pi R^2 \frac{sin(GR)}{GR}$$

Here we used definition of δ function

$$\int_a^b \delta(x - c)f(x) = \begin{bmatrix} f(c)\ if\ c\ \in\ [a;b] \\ 0 \quad if\ c\ \notin\ [a;b] \end{bmatrix}$$

d. It easy to note that plane $(2\,0\,0)$ has all even and plane $(1\,1\,1)$ has all odd indexes. Then the structure factor for those planes are $4f$, where f is an atomic form factor. Thus the ratio between diffraction peak intensities would be

$$\left(\frac{S_{200}}{S_{111}}\right)^2$$

This ratio can be evaluated by using the result of previous problem and having:

For $(2\,0\,0)$, $G = 2 \cdot |b1| = 2 \cdot 2\pi/a = 0.89\,\text{Å}^{-1}$

For $(1\,1\,1)$, $G = \sqrt{3} \cdot 2\pi/a = 0.77\,\text{Å}^{-1}$

$$\left(\frac{S_{200}}{S_{111}}\right)^2 = \left(\frac{sin(0.89 \cdot 3.5) \cdot 0.77}{sin(0.77 \cdot 3.5) \cdot 0.89}\right)^2 = \left(\frac{0.02}{0.38}\right)^2 \approx 0.003$$

The calculation shows that the $(2\,0\,0)$ peak should be very weak in the diffraction spectrum.

3) Thermal properties of metal (20 points).

a. Calculate 3D density of states $D(\omega)$ for phonons in a cubic crystal with size $L \times L \times L$. Use Debye approximation for dispersion relation $\omega = vk$. **(6 pt.)**

b. Calculate the number of phonons n_{ph} in this crystal. Show its dependence on temperature T in the two limiting cases: when $k_B T \gg \hbar\omega$ and when $k_B T \ll \hbar\omega$. **(6 pt.)**

c. Thermal conductivity coefficient in metal is given by $k \approx k_e = \frac{1}{3} C_e v l = \frac{\pi^2 N k_B^2}{3m} \tau T$.

Here electron scattering rate mainly due to interaction with phonons or impurities:

$\frac{1}{\tau} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_i} + \cdots$. Sketch k as a function of T. **(4 pt.)**

d. Also discuss and sketch how electrical conductivity in metal depends on temperature T. **(4 pt.)**

Solution

a. Density of states of phonons can be calculated using

$$D(\omega) = \frac{\partial N}{\partial k} \cdot \frac{\partial k}{\partial \omega}$$

where $\frac{\partial N}{\partial k} = \frac{L^3}{(2\pi)^3} 4\pi k^2$ is the number of states in the interval $k \to k + \Delta k$ in 3D space.

Using dispersion relation of acoustic wave for small k's $\omega = vk$ we can find that $\frac{\partial k}{\partial \omega} = \frac{1}{v}$ and

$$D(\omega) = \frac{L^3}{(2\pi)^3} 4\pi \frac{\omega^2}{v^3}$$

b. $n_{ph} = \int_0^{\omega_D} D(\omega)\langle n(\omega)\rangle d\omega$, where ω_D is Debye frequency.

$$n_{ph} = \frac{L^3}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^2}{exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$

In case $k_B T \gg \hbar\omega$ we can use Taylor expansion of the exponent in denominator

$$n_{ph} = \frac{L^3}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^2}{1 + \frac{\hbar\omega}{k_B T} - 1} d\omega = \frac{L^3 k_B \omega_D^2}{4\pi^2 v^3 \hbar} \cdot T$$

Which means that number of phonons is linearly proportional to the temperature when $k_B T \gg \hbar\omega$.

In case of $k_B T \ll \hbar\omega$ we can get

$$n_{ph} = \frac{L^3}{2\pi^2 v^3} \cdot \left(\frac{k_B T}{\hbar}\right)^2 \int_0^{\omega_D} \frac{\left(\frac{\hbar\omega}{k_B T}\right)^2}{exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$

here we can change the variables in the following way

$$\frac{\hbar\omega}{k_B T} = x$$

$$d\omega = \frac{k_B T}{\hbar} dx$$

$$\int_0^{\omega_D} d\omega \to \int_0^{x_D} dx$$

Than we can get such an integral

$$n_{ph} = \frac{L^3}{2\pi^2 v^3} \cdot \left(\frac{k_B T}{\hbar}\right)^3 \int_0^{x_D} \frac{x^2}{exp(x) - 1} dx$$

$k_B T \ll \hbar\omega$ means that $x \gg 1$ and integral can be simplified to the form of gamma function $\Gamma(n + 1) = \int_0^\infty x^n e^{-x} dx$

$$n_{ph} = \frac{L^3}{2\pi^2 v^3} \cdot \left(\frac{k_B T}{\hbar}\right)^3 \int_0^{x_D} x^2 exp(-x) dx = \frac{L^3}{2\pi^2 v^3} \cdot \left(\frac{k_B}{\hbar}\right)^3 \Gamma(3) \cdot T^3$$

Here we assumed that $\omega_D, x_D \to \infty$. Thus, number of phonons is proportional to T^3 at low temperatures.

c. Since $k_e = \frac{\pi^2 N k_B^2}{3m} \tau T$ we can use the fact that scattering rate of electrons with phonons is proportional to the number of phonons in the system $\frac{1}{\tau_{ph}} \propto n_{ph}$

Thus, we can distinguish several temperature regions:
1. High temperatures, where $n_{ph} \propto T \to k_e = const$

2. Intermediate regime, $n_{ph} \propto T^3 \to k_e \propto \frac{1}{T^2}$ In this two regimes scattering with phonons is a dominant process

3. Low temperature regime, when number of phonons becomes small, scattering is mainly due to impurities. One can note that number of impurities is a fixed number $\frac{1}{\tau_i} = const \to \tau = const \to k_e \propto T$
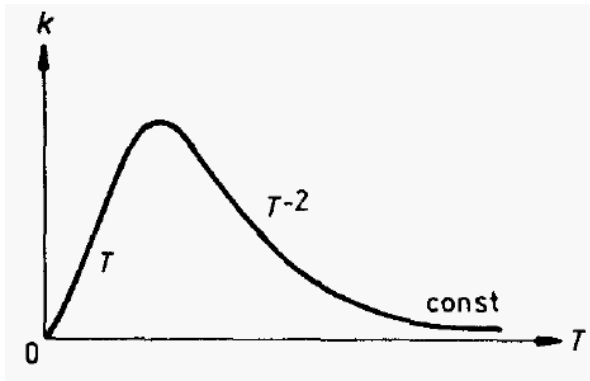
d. Noting that $\sigma = \frac{ne^2}{m^*} \cdot \tau$ we can use similar logic as in **c.** to find that at

1. High temperatures $\sigma \propto \frac{1}{T}$

2. Intermediate regime $\sigma \propto \frac{1}{T^3}$

3. Low temperature $\sigma = const$
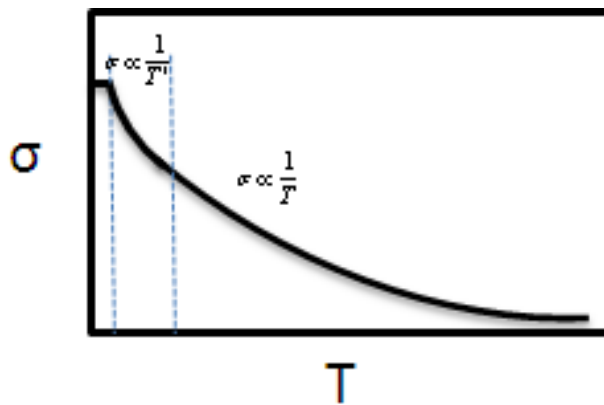
4) Hall effect (25 points).

a. Consider a specimen (see figure) in a longitudinal electric field E_x and a transverse magnetic field $B = B_z$. Write down equations of motion of electrons in this specimen, and find steady state solutions for electron velocities in all three dimensions. **(6 pt.)**

b. The Hall coefficient is defined by $R_H = \frac{E_y}{j_x B}$, derive the expression for R_H as a function of electron concentration n. **(8 pt.)**

c. Now assume there are two types of carriers in this specimen, electrons and holes, like in the case of a semiconductor material. Show $R_H = \frac{1}{e} \cdot \frac{p - nb^2}{(p + nb)^2}$, where n is electron concentration, p is hole concentration, and $b = \frac{\mu_e}{\mu_h}$ is the electron-hole mobility ratio. **(8 pt.)**

d. What do you expect the R_H will be for a material where $m_e = m_h$ and $p = n$? **(3 pt.)**
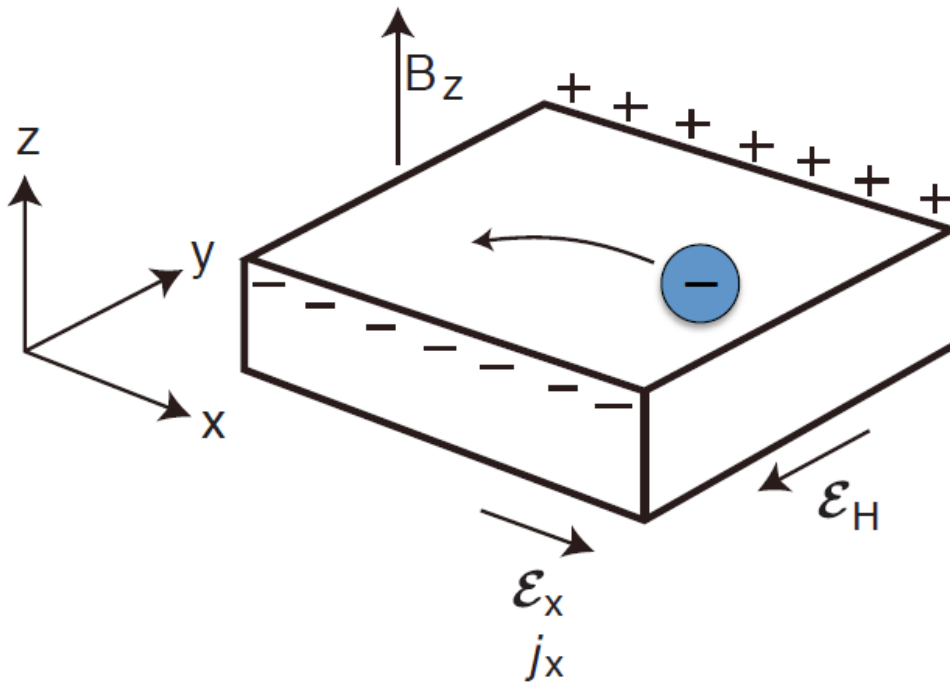
Solution

a. Electron in electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{B}$ experience a Lorentz force $\boldsymbol{F} = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$ in SI units. The static magnetic field B lie along the z axis. Than the component equations of motion are

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_x = -e(E_x + Bv_y);$$

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_y = -e(E_y - Bv_x);$$

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_z = -eE_z.$$

In the steady state in a static electric field the time derivatives are zero, so that the drift velocity is

$$v_x = -\frac{e\tau}{m}E_x - \cancel{\omega_c\tau v_y}$$

$$v_y = -\frac{e\tau}{m}E_y + \omega_c\tau v_x$$

$$v_z = -\frac{e\tau}{m}E_z$$

Where $\omega_c = eB/m$ is the cyclotron frequency.

b. The quantity defined by $R_H = \frac{E_y}{j_x B}$, where $j_x = -nev_x = ne^2\tau E_x/m$. (Note that the second term is omitted, movement in y direction doesn't influence x component of electron velocity, its driven by electric field only, so-called drift velocity approximation). Than

$$R_H = -\frac{\dfrac{eB\tau E_x}{m}}{\dfrac{ne^2\tau BE_x}{m}} = -\frac{1}{ne}$$

c. In analogous way we can write the equations of motion for electrons and holes in magnetic field and find components of velocity

For electrons

$$v_x = -\frac{e\tau}{m}E_x - \cancel{\omega_c \tau v_y}$$

$$v_y = -\frac{e\tau}{m}E_y + \omega_c \tau v_x$$

$$v_z = -\frac{e\tau}{m}E_z$$

For holes

$$v_x = \frac{e\tau}{m}E_x + \cancel{\omega_c \tau v_y}$$

$$v_y = \frac{e\tau}{m}E_y - \omega_c \tau v_x$$

$$v_z = \frac{e\tau}{m}E_z$$

Assumption was made that x component of velocity is not influenced by y movement of charge, it is driven only by electric field. Thus, the total contribution to x component of current density is

$$j_x = j_x^e + j_x^h = (ne\mu_e + pe\mu_h)E_x$$

Similarly we can find an expression for y component of current density for both types of carriers as

$$j_x^e = ne\mu_e\left(E_y + \mu_e B E_x\right) \text{ for electrons}$$
$$j_x^h = pe\mu_h\left(E_y - \mu_h B E_x\right) \text{ for holes}$$

Using $j_y = j_y^e + j_y^h = 0$ we can derive that

$$E_y = E_x B \frac{p\mu_h^2 - n\mu_e^2}{p\mu_h + n\mu_e} \qquad (SI)$$

Than

$$R_H = \frac{E_y}{j_x B} = \frac{1}{e} \cdot \frac{p - nb^2}{(p + nb)^2} \qquad (SI)$$

Where $b = \frac{\mu_e}{\mu_h}$

d. R_H expected to be 0, this can happen in fully compensated semimetal where both carrier concentrations are the same.

5) Semiconductor and superconductor properties (20 points).

a. Describe the difference between *insulator*, *semiconductor*, *semimetal* and *metal*. **(4 pt.)**

b. $p - n$ junction **(10 pt.)**
   i. Explain the concept of p and n type semiconductors,
   ii. Draw the schematic energy diagram.
   iii. What will happen on the interface if you now bring them in contact?
   iv. Draw the energy levels at the interface before and after diffusive equilibrium is established.
   v. Based on the energy diagram explain how a solar cell works.

c. Qualitatively explain the physical phenomena shown on the picture below. **(6 pt.)**

Solution

a. See Kittel 8th ed. P. 162. Fig. 1
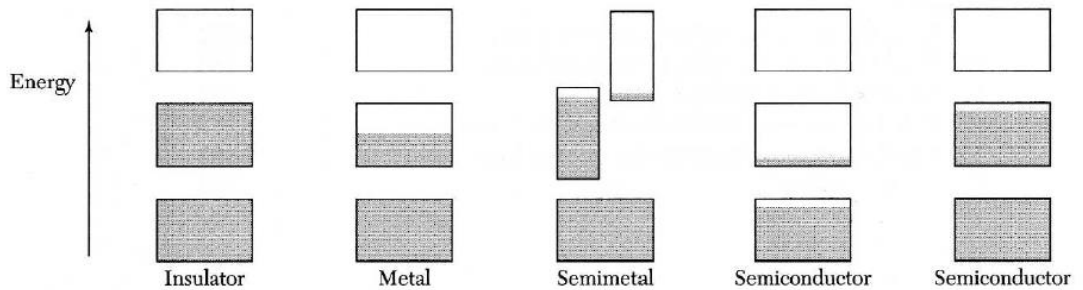
Schematic electron occupancy of allowed energy bands for an insulator, metal, semi-metal, and semiconductor. The vertical extent of the boxes indicates the allowed energy regions; the shaded areas indicate the regions filled with electrons. In a **semimetal** (such as bismuth) one band is almost filled and another band is nearly empty at absolute zero, but a pure **semiconductor** (such as silicon) becomes an insulator at absolute zero. The left of the two semiconductors shown is at a finite temperature, with carriers excited thermally. The other semiconductor is electron-deficient because of impurities.

b. i) n and p are electron/hole doped semiconductors with Fermi level shifted towards the conduction/valence band.
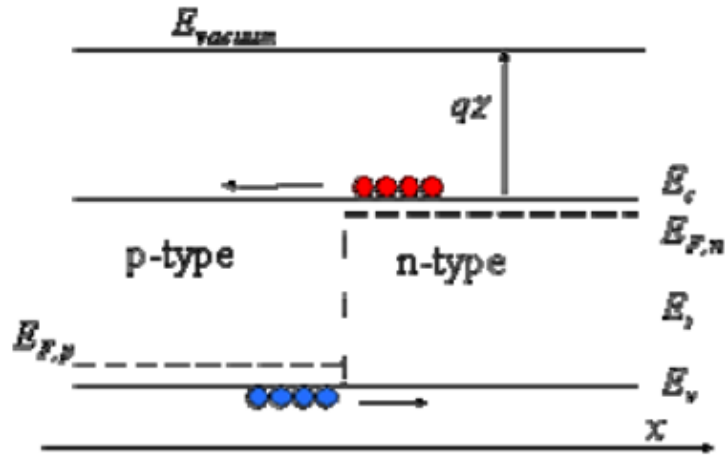
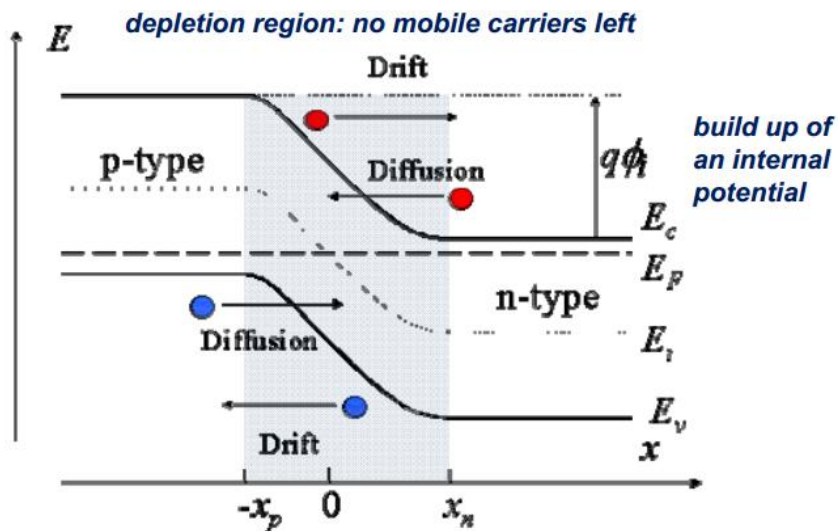ii) Corresponding energy diagram of p and n semiconductors:
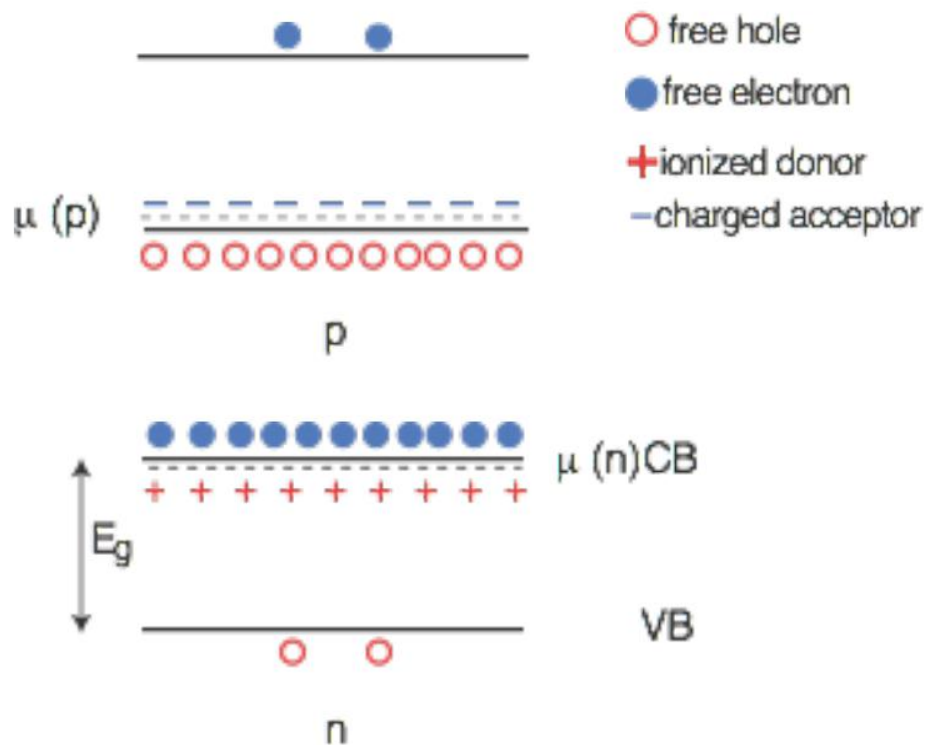
iii) Fermi levels on both sides will be alliged at the interface. Build-in electric field will be established opposite to the charge movement. It will decay if
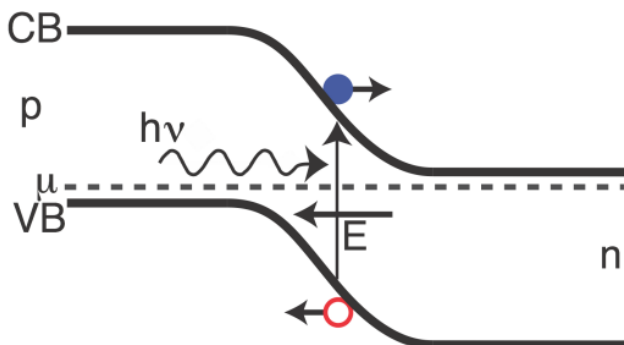
one moves away from the interface.

iv) Before equilibrium:

After equilibrium is established:

v) If the *p-n* junction is illuminated by light with frequency larger than the bandgap of semiconductor electron-hole (exciton) pair will be generated within the depletion region. Later it can be broken and driven by build-in electric field.

Voltage will be generated on the two end of junction. Typical $I - V$ characteristic of solar cell integrated into a simple circuit under light illumination is shown on the picture.
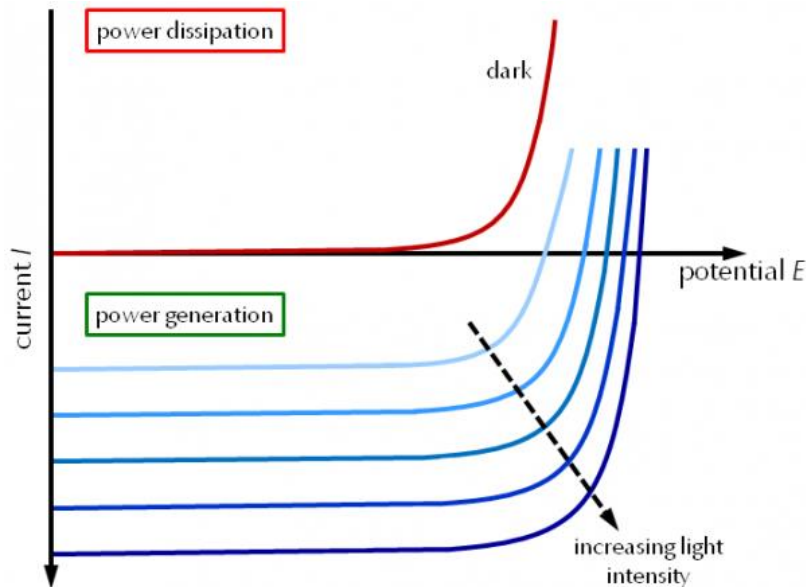
Without light it recovers typical $p - n$ junction $I - V$ characteristic.

c. The phenomena shown on the picture is Meissner effect. When a superconductor is cooled down below its critical temperature in applied magnetic field the magnetic flux originally present in the material will be ejected. In this way position of superconductor can be "locked" in space by magnetic field. In some extreme cases when superconductor can withstand large magnetic field it becomes possible to carry extra weight. This is an example of perfect diamagnetism.
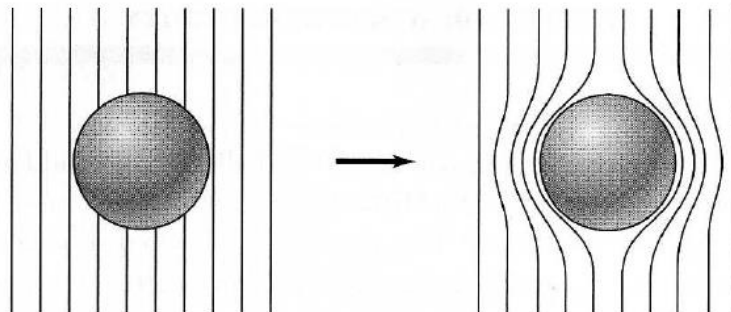

Figure 2 Meissner effect in a superconducting sphere cooled in a constant applied magnetic field; on passing below the transition temperature the lines of induction **B** are ejected from the sphere.