

Module IV

Practical assignments:

1. A two-dimensional 1x1 cm metallic sample consists of monovalent atoms crystallized in a simple rectangular primitive cell having parameters $a = 2\text{\AA}$ and $b = 4\text{\AA}$. Calculate and make a scaled drawing of the 1st Brillouin zone and the free electron Fermi sphere. Elaborate why and how the situation changes for the case of nearly free electrons and make a corresponding drawing.

2. Consider a 2D graphene sheet. The primitive vectors of the Bravais lattice are given by $\vec{a}_1 = \left(\frac{3a}{2}\right)\vec{e}_x + (\sqrt{3}a/2)\vec{e}_y$ and $\vec{a}_2 = \left(\frac{3a}{2}\right)\vec{e}_x - (\sqrt{3}a/2)\vec{e}_y$, where $a = 0.142\text{nm}$. The energy bands of the graphene sheet are found to be given by

$$E_{c,v}(\vec{k}) = \pm t \left[1 + 4 \cos \sqrt{3} k_y a/2 \cos \frac{3k_x}{2} + 4 \cos^2 \sqrt{3} k_y a/2 \right]^{1/2}$$

with $t = 3\text{ eV}$.

(a) Plot $E_{c,v}(\vec{k})$ along $[10]$, $[01]$, and $[11]$ directions. Indicate the band gap.

(b) Derive a general expression for the effective mass of electrons in the conduction band of the graphite sheet. Find its values at the Γ point and $[01]$ edge of the 1st BZ.

3. GaAs is a semiconductor with a direct band gap of $\sim 1.42\text{ eV}$ at room temperature. The experimental values for the effective masses (in unit of the free electron mass) are: 0.067, 0.082, and 0.45 for electrons in the conduction band as well as light and heavy holes at the top of the valence bands, respectively. Compute the corresponding energy dispersion relations and sketch the band structure of GaAs in the vicinity of Γ point. What is the origin to have “light” and “heavy” holes?
4. Consider P donors in Si in terms of hydrogen-like model in the effective mass approximation.
 - (a) Calculate the value of the ionization level for electrons to be excited to the conduction band;

(b) calculate the Borh orbit for these electrons and estimate the doping concentration to transform localized states into an impurity band.

5. Consider the carrier concentration evolution as a function of temperature in 10^{17} P/cm^3 homogeneously doped Si. Choose several characteristic temperature limits, specifically low, intermediate, and high – corresponding to the donor freezing out, full donor activation, and overtaking by intrinsic carriers, respectively. For these limits, compute
- (a) the equilibrium concentration for electrons and holes;
 - (b) the E_F position relative to E_i ;

Plot the electron concentration and E_F position as a function of temperature ($1/T$).