Introduction to Physics of Nanoparticles and Nano structures[1]

Part II: Physics of Nanostructures: **Questions on Module 1**

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1. What is the difference between Diamond and Zinc Blende structures? Consider a cubic cell with sides equaling the lattice constant a_o, in the first quadrant and one corner of cubic cell as origin. Enlist the coordinate locations of the sites (taking the cell in the first quadrant) for the two structures to distinguish them.

2. Give examples of semiconductors with reference to the periodic table, and enlist them in tabular form.

3. Explain what is valley degeneracy for indirect gap semiconductors, with examples.

4. From the so called **k.p** method of band structure calculations, it can be shown that for direct gap semiconductors, the effective mass m_e^* of conduction electrons is given by

$$\frac{m_e}{m_e^*} = 1 + \frac{2P^2}{m_e E_g},$$

where m_e is the bare electron mass, E_g is the energy gap of the semiconductor, and $P \approx 2\pi\hbar/a_o$ with a_o denoting the lattice constant. Assuming Vegard's law for a_o and rigid band model for E_g, obtain an expression for m_e^*/m_e as a function of x for small x for the alloy A_xB_{1-x} of two semiconductors A and B, which have nearly same lattice constants.

5. The density of states (DOS) $D(E)$ for conduction band electrons in 3-dimension is defined via
$D(E)dE$ = the total number of states (including spin degeneracy) per unit volume in the energy interval E to $E + dE$.
Show that near the bottom of the conduction band where the electron energy spectrum is given by $E(k) = E_c + \hbar^2k^2/(2m_e^*)$, the DOS is given by

$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}, \qquad E \geq E_c.$$

Why and how is the formula modified for a indirect gap semiconductor?

6. Show that near the top of the valence band where the electron energy spectrum is given by $E(k) = E_v - \hbar^2k^2/(2m_{hh}^*)$ for heavy holes and $E(k) = E_v - \hbar^2k^2/(2m_{lh}^*)$ for light holes, the DOS is given by

$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m_{dos}^*}{\hbar^2}\right)^{3/2}\sqrt{E_v - E}, \qquad E \leq E_v,$$

where m_{dos}^* is the DOS effective mass for the holes; explain and derive the formula for the m_{dos}^*.

7. Show that when Boltzmann approximation is applicable, the electron carrier concentration n in the conduction band of a semiconductor at temperature T is given by

$$n = N_c e^{\beta(\mu - E_c)},$$

[1] Instructor: Prof. G. Mukhopadhyay, Physics Department, IIT Bombay, Mumbai-400076, India.

where μ is the chemical potential of the electrons, E_c is the conduction band energy minimum, $\beta = 1/(k_B T)$, and N_c is the so called effective density of states at the conduction band edge, given by

$$N_c = 2\left(\frac{2m^*_{dos} k_B T}{2\pi\hbar^2}\right)^{3/2}.$$

Calculate the value of N_c in cm^{-3} taking $m^*_{dos} = m_e$ and $T = 300$ K.

8. Similarly show that when Boltzmann approximation is applicable, the hole carrier concentration p in the valence band of a semiconductor at temperature T is given by

$$p = N_v e^{\beta(E_v - \mu)},$$

where E_v is the valence band energy maximum, and N_v is the so called effective density of states at the valence band edge, given by the same expression as N_c, but with m^*_{dos} now denoting the DOS effective mass for the holes.

9. Using the results of the last two problems, show that under the Boltzmann approximation,

$$np = N_c N_v e^{-\beta E_g},$$

where $E_g = E_c - E_v$ is the energy gap for the semiconductor, so that the carrier densities in intrinsic semiconductors are given by

$$n_i = p_i = \sqrt{N_c N_v} e^{-\beta E_g/2} = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m^*_e m^*_h)^{3/4} e^{-\beta E_g/2}.$$

where the effective masses refer to the DOS effective masses. Also show that for intrinsic semiconductors, the chemical potentialμ_i is given by

$$\mu_i = (E_c + E_v)/2 + (3/4) k_B T \ln(m^*_h/m^*_e).$$

10. An electron of charge $-e$ donated by an impurity that donates one electron per atom in a semiconductor of dielectric permittivity ε, sees the potential due to the positive ion left behind, so that its potential energy is given by

$$U(\vec{r}) = -\frac{e^2}{4\pi\varepsilon}\frac{1}{r}.$$

Show that the ground state energy of the donor level E_d is given by

$$E_d = -\left(\frac{m^*_e}{m_e}\right)\left(\frac{\varepsilon_o}{\varepsilon}\right)^2 \times 13.6\,\text{eV},$$

below the bottom of the conduction band E_c, where m^*_e is m^*_σ, the effective mass for transport of conduction electrons, e.g., for indirect gap semiconductors, $m^*_\sigma = 3/(2/m^*_t + 1/m^*_l)$.

11. Similarly, show that the acceptor level for an acceptor impurity that captures one electron per impurity atom, has its ground state energy given by

$$E_a = +\left(\frac{m^*_h}{m_e}\right)\left(\frac{\varepsilon_o}{\varepsilon}\right)^2 \times 13.6\,\text{eV},$$

above the top of the valence band E_v.

12. In a semiconductor, the electron and hole can interact to produce a electron-hole pair bound state called exciton. Using the Effective Mass Approximation, show that the ionization energy of exciton is given by $E_x = R^*$, where R^* is the so called excitonic Rydberg energy.

13. In an intrinsic semiconductor at a given temperature T, there is a thermal equilibrium between excitons and the free electron and hole pairs. If the concentrations are n_x for the excitons, and $n_e = n_h = n$ for the free electrons or the holes, then show that

$$n_x = n^2 \left(\frac{2\pi\hbar^2}{\mu k_B T}\right)^{3/2} e^{\beta R^*},$$

where μ is the electron-hole reduced mass, and $\beta = 1/(k_B T)$.

14. A compensated semiconductor has donor impurities of concentration N_d, as well as acceptor impurities of concentration N_a. If all impurities are ionized, derive the expressions for the carrier concentrations n_e for a n-type and n_p for a p-type semiconductor.

15. Using the statistics for donors, determine the fraction $n_d/(n_d+n_e)$, where n_d is the concentration of unionized donors. Similarly, using the statistics for acceptors, determine the fraction $n_a/(n_a + n_p)$, where n_a is the concentration of unionized acceptors.

16. Show that for a compensated semiconductor, the difference in chemical potentials for electron and hole is given in Boltzmann approximation by

$$\mu_e - \mu_h = E_g + k_B T \ln\left(\frac{n_e n_p}{N_c N_v}\right).$$

References:

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