Assignment 5

EE 698N, Advanced Semiconductor Physics
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1 Optical transitions: Allowed and Forbidden Absorption

We derived the absorption coefficient for ALLOWED transitions for a 2-band direct-bandgap semiconductor. We found that the absorption coefficient to be (in cm^{-1})

$$\alpha_{allowed} = 2.7 \times 10^5 (\frac{2m_r}{m})^{\frac{3}{2}} \frac{f}{\eta} \sqrt{\hbar\omega - E_g} \tag{1}$$

Here $f \approx 1 + m/m_h$ is the dimensionless oscillator strength, and η is the refractive index of the semiconductor.

In this problem, you will derive the absorption coefficient for a FORBIDDEN transition in a direct bandgap semiconductor. Follow the handouts closely for this problem.

a) Find the matrix element $H_{k'k}$ for absorption of a photon whose vector potential is given by $\mathbf{A} = \mathbf{a}Ae^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$. Use Bloch-functions as eigenstates for electrons in the initial (valence band) and final (conduction band) states. Show that it is composed of two terms, one leading to direct, and the other to indirect transitions.

b) Show that the probability of forbidden transition is proportional to $|\mathbf{a}\cdot\mathbf{k}|^2$, where $\mathbf{k}$ is the wavevector of the electron in the valence band. Since $\mathbf{a}$ is a constant unit vector, show that the average value of $|\mathbf{a}\cdot\mathbf{k}|^2$ over the Brillouin Zone is $k^2/3$.

c) Show that the resulting absorption coefficient $\alpha = r/\Phi$ where r is the rate of forbidden absorption per unit volume of the semiconductor, and $\Phi = \langle\mathbf{S}\rangle/\hbar\omega$ is the photon flux is given by (Eq. 7.70)

$$\alpha = \frac{q^2(2m_r)^{\frac{5}{2}}f'}{6\pi\epsilon_0\eta c m^2\hbar^2} f_0(1-f_0)\frac{(\hbar\omega - E_g)^{3/2}}{\hbar\omega}. \tag{2}$$

d) There is a printing error in Equation 7.68 (in the handouts on optical properties) in the derivation of the absorption coefficient for forbidden transitions. Confirm this by dimensional analysis. What is the error?

2 Optical Transitions: The Quantum-Confined Stark Effect

We saw in class that an electric field can cause transitions below the bandgap in a bulk direct-gap semiconductor (the Franz-Keldysh effect). A similar effect occurs when an electric field is applied across a quantum well.

The Stark shift of the confined levels in a quantum well can be calculated by using second-order perturbation theory. Consider the interaction between the electrons (effective mass $m^\star$) in a quantum well of width d and a DC electric field of strength F_z applied along the z (growth) axis.

a) Explain why the perturbation to the energy of an electron is given by $H' = eF_z z$. Draw a band diagram to depict the situation.

b) Explain why the first-order shift of the energy levels, given by

$$\Delta E_n^{(1)} = \int_{-\infty}^{+\infty} dz \phi_n^\star(z) H' \phi_n(z) \tag{3}$$

is ZERO.

c) The second-order energy shift of the $n = 1$ level [1] is given by

$$\Delta E_{n=1}^{(2)} = \sum_{n>1} \frac{|\langle 1|H'|n\rangle|^2}{E_1 - E_n}, \tag{4}$$

where

$$\langle 1|H'|n\rangle = \int_{-\infty}^{+\infty} dz \phi_1^\star(z) H' \phi_n(z). \tag{5}$$

Show that for an electron in a quantum well with infinitely high barriers, the Stark shift is given approximately by

$$\Delta E = -24(\frac{2}{3\pi})^6 \frac{e^2 m^\star d^4}{\hbar^2} F_z^2. \tag{6}$$

d) Note that the QCSE-shift goes as $\Delta E \sim m^\star d^4 F_z^2$. Calculate and plot the shift (in meV) for a $d = 10nm$ thick AlGaAs/GaAs/AlGaAs quantum well as a function of electric fields over a range typical in semiconductor devices. Comment on how this shifts the interband transition wavelength (red or blue?) by using same arguments for holes.

3 Lyddane-Sachs-Teller Relation, Restrahlen Band

When an electromagnetic wave interacts with the optical phonons (TO, LO) in a semiconductor, various fundamental properties emerge. The dielectric constant of the semiconductor, which is a measure of the "screening" of an electric field applied across a semiconductor, becomes dependent upon the frequency of the EM wave.

a) Prove the Lyddane-Sachs-Teller (LST) relation

$$\frac{\epsilon_r(0)}{\epsilon_r(\infty)} = (\frac{\omega_{LO}}{\omega_{TO}})^2, \tag{7}$$

and the corresponding frequency-dependent dielectric constant

$$\epsilon_r(\omega) = \epsilon_r(\infty) \frac{\omega_{LO}^2 - \omega^2}{\omega_{TO}^2 - \omega^2}. \tag{8}$$

Plot the dielectric constant as a function of the frequency of incident EM wave frequency, alongside the reflectivity[2].

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[1] Note the similarity to what we did in $\mathbf{k} \cdot \mathbf{p}$ theory due to interaction between the $n = 1$ state with all other states through the perturbation potential. This interaction led to the conclusion that the effective mass of CB electrons is proportional to the bandgap.

[2] Reflectivity is given by $R = |\frac{\sqrt{\epsilon_r} - 1}{\sqrt{\epsilon_r} + 1}|^2$

b) Show that as a result of the negative $\epsilon_r(\omega)$ for $\omega_{TO} \leq \omega\omega_{LO}$, EM waves within this narrow band of energies suffer strong reflection when normal-incident on a semiconductor surface. Such bands are called 'Restrahlen', a German word meaning "residual rays". Light in the Restrahlen band cannot propagate in the medium, and is reflected back.

c) Figure 1 shows the measured reflectivity of an AlSb sample[3].

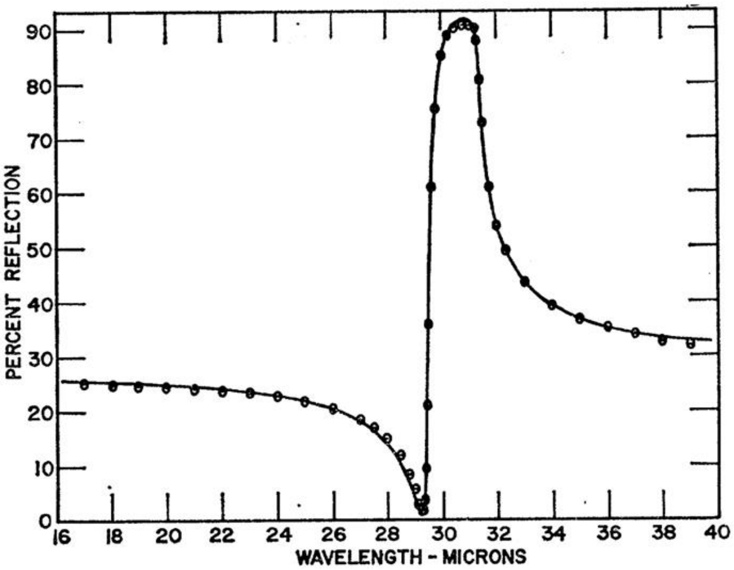

Figure 1: Experimentally measured reflectivity from a AlSb crystal

Use the data to estimate the four fundamental quantities $\omega_{LO}, \omega_{TO}, \epsilon_r(0), \&\epsilon_r(\infty)$. Express the TO and LO phonon energies you extract from the experimental data in meV. Compare your calculations to those in semiconductor datasheets.

d) Can you explain why metals are good reflectors of visible wavelengths? Sketch the expected reflectivity vs photon energy plot for a typical metal.

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[3] From Phys. Rev. vol 127, pg 126