MSE 5460/ECE 5570, Spring Semester 2016
Compound Semiconductors Materials Science

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Assignment 2

Policy on assignments: Please turn them in by 5pm, **Wednesday, March 9th, 2016**.

General notes: Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. BOX your final answers where applicable. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover.

Problem 2.1) Si and Compound Semiconductor Bandstructure Symmetries

a) In Assignment problem **1.4** you obtained the LCAO bandstructure of the compound semiconductor GaAs. From the 8×8 LCAO matrix, show that for the Γ point with $\mathbf{k} = 0$, the eight eigenvalues can be calculated analytically. Then prove that for GaAs, the conduction band edge state is at $E_c(\Gamma) = \frac{E_s^{Ga}+E_s^{As}}{2} + \sqrt{(\frac{E_s^{Ga}-E_s^{As}}{2})^2 + (4V_{ss\sigma})^2}$ composed of $|s\rangle$ orbital overlap between the Ga and As atoms, and no $|p\rangle$ orbitals are involved.

b) Similarly, show that for the states at the top of the valence band at the Γ point, only $|p\rangle$ orbitals are involved with no $|s\rangle$ orbital involvement. Use this property to argue why holes are anisotropic in most compound semiconductors, but electrons are isotropic.

c) Solve **Rockett problem 5.7.4** (MSS Page 233).

Problem 2.2) Density of States of Electrons, Photons, and Phonons

a) Show that for a parabolic bandstructure for electrons $E(k) = E_c + \frac{\hbar^2 k^2}{2m^\star}$ with band edge E_c and effective mass $m^\star$, the DOS for electron motion in d dimensions is $\boxed{g_d(E) = \frac{g_s g_v}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2})} (\frac{2m^\star}{\hbar^2})^{\frac{d}{2}} (E - E_c)^{\frac{d}{2}-1}}$. Sketch the DOS for 3D, 2D, and 1D electron systems using the expression. Explain the roles of the valley degeneracy and the effective mass for Silicon and compound semiconductors. [Here $\Gamma(...)$ is the Gamma function with property $\Gamma(x+1) = x\Gamma(x)$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. You may need the expression for the surface area of a $d-$dimensional sphere in $k-$space: $S_d = \frac{2\pi^{\frac{d}{2}} k^{d-1}}{\Gamma(\frac{d}{2})}$. Check that this reduces to the surface area of a sphere for $d = 3$ and the circumference of a circle for $d = 2$.]

b) Solve **Rockett problem 2.6.6** (MSS Page 70).

c) Show that the DOS for energy dispersion $E(k) = \hbar v k$ for 3 dimensions is $\boxed{g_\omega(\omega) = \frac{g_p \omega^2}{2\pi^2 \hbar v^3}}$, where $\omega = vk$, and g_p is the polarization degeneracy. This is the dispersion for *waves*, such as photons and phonons moving with velocity v. The parabolic DOS of phonons and photons will play an important role in the thermal and photonic properties of semiconductors.

Problem 2.3) Quantized Electronic States in Compound Semiconductor Heterostructures

We discussed in class the finite quantum well problem as the basis of all quantized structures based on compound semiconductor heterostuctures. In this problem you evaluate some examples to gain insight, and collect some *very* useful formulae for the quantum design of heterostructure devices.

a) With relevant formulae and sketches, outline the graphical method for identifying the bound state eigenvalues and eigenfunctions in a finite quantum well of height U_0 and width L_w for a quantum well semiconductor material with effective mass $m^\star$. Show that the solution for allowed k values take the form $\sqrt{\frac{\theta_0^2}{\theta^2} - 1} = \tan\theta$ and $\sqrt{\frac{\theta_0^2}{\theta^2} - 1} = -\cot\theta$, where $\theta = \frac{kL_w}{2}$, and the characteristic constant $\theta_0^2 = \frac{m^\star L_w^2 U_0}{2\hbar^2}$.

b) Show that in the case of a vanishingly small barrier height $U_0 \to 0$, there is still at least one bound state for the 1D quantum well with a *binding energy* equal to $\boxed{U_0 - E_1 \approx \theta_0^2 U_0}$.

c) Show that the number of bound states is $\boxed{N = 1 + \text{Int}[\frac{2\theta_0}{\pi}]}$, where Int$[x]$ is the largest integer smaller than x. Show that the numerical value is $N = 1 + \text{Int}[1.63(\frac{L_w}{1 \text{ nm}})\sqrt{(\frac{m_0}{m^\star}) \cdot (\frac{U_0}{1 \text{ eV}})}]$.

d) Solve **Rockett problem 2.6.4** (MSS Page 70) to apply the above results for a GaAs/AlGaAs quantum well.

e) Will an *asymmetric* 1D well with different barrier heights on both sides also be guaranteed one bound state? What sort of a 1D well will have no bound states?

Problem 2.4) Compound Semiconductor Heterostructure Quantum Design

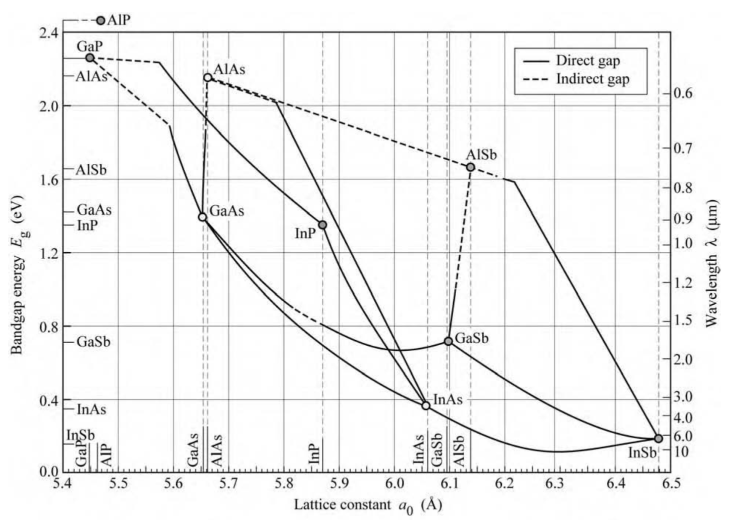

Figure 1: Bandgaps and Lattice Constants of Compound Semiconductors (From Schubert's book on LEDs).

As the CTO of the stealth startup 'The Quantum Mechanics' you win a project from NASA to design an infrared photodetector for the detection of a very weak $\lambda_0 = 12.4$ μm radiation from a distant star. Because you have in your team the world's best group of III-V compound semiconductor MBE growers who can grow for you layered heterostructures of any combination of materials you can dream up from Figure 1, you decide the design will be done using *intersubband transitions* in III-V quantum wells. Describe your design in quantitative detail - including plots, choices of materials, thicknesses, etc. Neglect selection rules for optical transitions, assume the 75%:25% $\Delta E_c : \Delta E_v$ band offset distribution, and use the rule of thumb that you cannot grow a strained layer thicker than $t_{cr} \sim \frac{a_0}{2\epsilon}$ where ϵ is the strain. [Use results of **Problem 2.3**.]