MIT 6.772/SMA 5111: COMPOUND SEMICONDUCTOR DEVICES
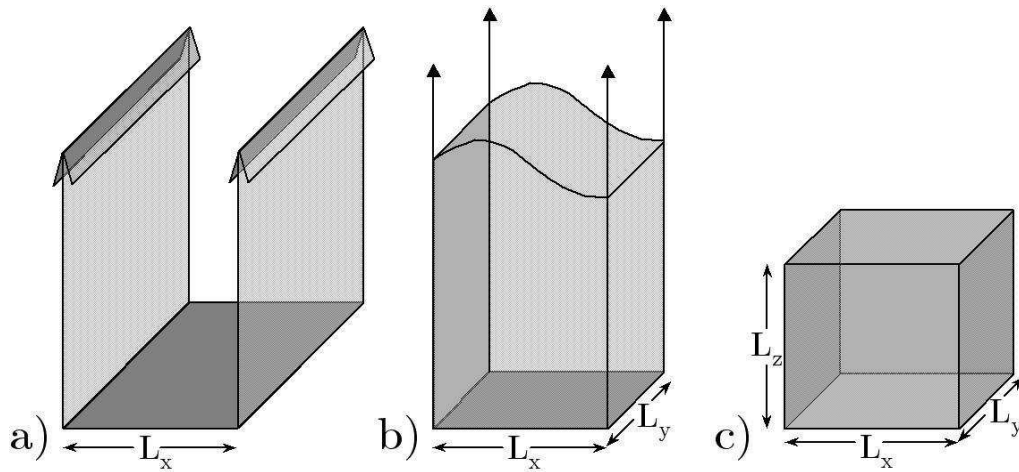
Problem Set No. 2 Solutions

Problem 2.1

Figure 1: a) Quantum Well, b) Quantum Wire, c) Quantum Dot. $L_x = L_y = L_z = 5 \pm 0.25 \ nm$.

Part a: Evaluate the ground state of a quantum well, $L_x = 5 \pm 0.25 \ nm$:

$$E_n = \frac{\hbar^2}{2 \cdot m} \left(\frac{\pi \cdot n}{L_x} \right)^2 \tag{1}$$

For the ground state ($n = 1$):

$L_x = 4.75 \ nm$	$L_x = 5.0 \ nm$	$L_x = 5.25 \ nm$
$E_1 = \frac{\hbar^2}{2 \cdot m} \left(\frac{\pi}{4.75 \ nm} \right)^2 = 0.238 \ eV$	$E_1 = \frac{\hbar^2}{2 \cdot m} \left(\frac{\pi}{5.0 \ nm} \right)^2 = 0.215 \ eV$	$E_1 = \frac{\hbar^2}{2 \cdot m} \left(\frac{\pi}{5.25 \ nm} \right)^2 = 0.195 \ eV$

Note that $E_n \propto L^{-2}$, so the uncertainty is different for $L_x = 4.75 \ nm$, and $L_x = 5.25 \ nm$.

$$E_1 \in [0.195 \ eV, \ 0.238 \ eV]$$

Part b: Evaluate the ground state of a quantum wire, $L_x = L_y = 5 \pm 0.25 \ nm$:

We will use the worst case (We will make L smallest in both directions to give the largest upper deviation, and the largest in both directions for give the lowest deviation).

$$E_{n,m} = \frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi \cdot n}{L_x}\right)^2 + \left(\frac{\pi \cdot m}{L_y}\right)^2\right]$$

For the ground state ($n = m = 1$):

$L_x = L_y = 4.75\ nm$	$L_x = L_y = 5.0\ nm$	$L_x = L_y = 5.25\ nm$
$E_{1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.476\ eV$	$E_{1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.43\ eV$	$E_{1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.39\ eV$

$$E_{1,1} \in [0.39\ eV,\ 0.476\ eV]$$

Part c: Evaluate the ground state of a quantum dot, $L_x = L_y = L_z = 5 \pm 0.25\ nm$:

Again, we will use the worst case (We will make L smallest in all directions to give the largest upper deviation, and the largest in all directions for give the lowest deviation).

$$E_{n,m,l} = \frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi \cdot n}{L_x}\right)^2 + \left(\frac{\pi \cdot m}{L_y}\right)^2 + \left(\frac{\pi \cdot l}{L_y}\right)^2\right]$$

For the ground state ($n = m = l = 1$):

$L_x = L_y = L_z = 4.75\ nm$	$L_x = L_y = L_z = 5.0\ nm$	$L_x = L_y = L_z = 5.25\ nm$
$E_{1,1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.714\ eV$	$E_{1,1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.645\ eV$	$E_{1,1,1} = 2 \cdot \frac{\hbar^2}{2 \cdot m}\left(\frac{\pi}{L_x}\right)^2 = 0.585\ eV$

$$E_{1,1} \in [0.585\ eV,\ 0.714\ eV]$$

Part d: Design a quantum wire such that the ground state is equal to the ground state of a quantum well, $L_{x,well} = 5\ nm$:

We will assume that $L_{x,wire} = L_{y,wire}$ for the quantum wire.

$$
\begin{aligned}
E_{1,well} &= E_{1,1,wire} \\
\frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi}{L_{x,well}}\right)^2\right] &= \frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi}{L_{x,wire}}\right)^2 + \left(\frac{\pi}{L_{y,wire}}\right)^2\right] \\
\frac{1}{L_{x,well}^2} &= \frac{2}{L_{x,wire}^2} \\
L_{x,wire} = L_{y,wire} &= L_{x,well}\sqrt{2} = 7.071\ nm
\end{aligned}
$$

Part e: Design a quantum dot such that the ground state is equal to the ground state of a quantum well, $L_{x,well} = 5\ nm$:

We will assume that $L_{x,dot} = L_{y,dot} = L_{z,dot}$ for the quantum dot.

$$
\begin{aligned}
E_{1,well} &= E_{1,1,1,dot} \\
\frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi}{L_{x,well}}\right)^2\right] &= \frac{\hbar^2}{2 \cdot m}\left[\left(\frac{\pi}{L_{x,dot}}\right)^2 + \left(\frac{\pi}{L_{y,dot}}\right)^2 + \left(\frac{\pi}{L_{z,dot}}\right)^2\right] \\
\frac{1}{L_{x,well}^2} &= \frac{3}{L_{x,dot}^2} \\
L_{x,dot} &= L_{y,dot} = L_{z,dot} = L_{x,well}\sqrt{3} = 8.66\ nm
\end{aligned}
$$

Problem 2.2

a: Sketch a P-n $Al_{0.4}Ga_{0.6}As$ and $GaAs$ heterojunction, $N_{AP} = 5 \times 10^{17} cm^{-3}$ and $N_{Dn} = 10^{17} cm^{-3}$:

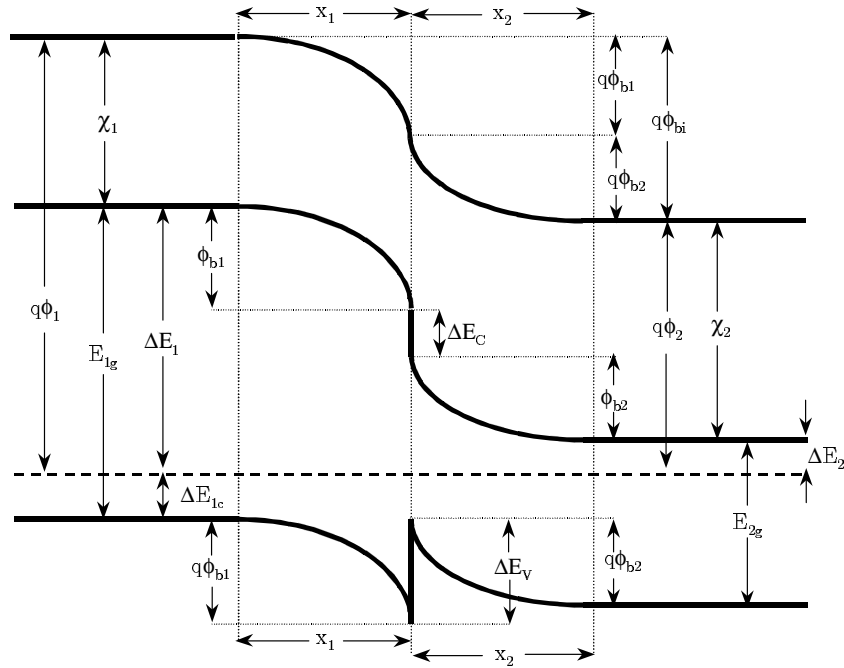|	$Al_{0.40}Ga_{0.60}As$	$GaAs$
$\chi \; [eV]$	3.63	4.07
$E_g \; [eV]$	1.92	1.42
ϵ_r	11.6	12.9
$N_C \; [cm^{-3}]$	5.0×10^{17}	4.7×10^{17}
$N_V \; [cm^{-3}]$	8.0×10^{18}	7.0×10^{18}
$N_A \; [cm^{-3}]$	5.0×10^{17}	$-$
$N_D \; [cm^{-3}]$	$-$	1.0×10^{17}

Figure 2: A P-n junction between $Al_{0.4}Ga_{0.6}As$ and $GaAs$.

$$\Delta E_g = E_{g,2} - E_{g,1} = -0.500 \; eV$$

$$\Delta E_{1,c} = \frac{k_B T}{q} ln\left(\frac{N_{V,1}}{N_{A,1}}\right) = 0.072 \; eV$$

$$\Delta E_1 = E_{g1} - \Delta E_{1,c} = 1.848 \; eV$$

$$\Delta E_2 = \frac{k_B T}{q} ln\left(\frac{N_{C,2}}{N_{D,2}}\right) = 0.040 \; eV$$

$$\Delta E_c = \chi_1 - \chi_2 = -0.440 \; eV$$

$$\Delta E_v = \Delta E_c - \Delta E_g = 0.060 \; eV$$

$$q\phi_1 = \chi_1 + \Delta E_1 = 5.478 \ eV$$

$$q\phi_2 = \chi_2 + \Delta E_2 = 4.11 \ eV$$

$$q\phi_{bi} = q\phi_2 - q\phi_1 = -1.368 \ eV$$

$$x_1 = \sqrt{\frac{2N_2 \cdot \epsilon_1 \cdot \epsilon_2 \cdot q\phi_{bi}}{q \cdot N_1 \left(\epsilon_1 N_1 + \epsilon_2 N_2\right)}} = 24.388 \ nm$$

$$x_2 = \frac{N_1}{N_2} x_1 = 121.939 \ nm$$

$$q\phi_{b1} = q\left[\frac{q}{2\epsilon_1} N_1 x_1^2\right] = 0.209 \ eV$$

$$q\phi_{b2} = q\left[\frac{q}{2\epsilon_2} N_2 x_2^2\right] = 1.160 \ eV$$

b: $N_{DN} = 2 \times 10^{17} cm^{-3}$ **and** $N_{Ap} = 6 \times 10^{17} cm^{-3}$:

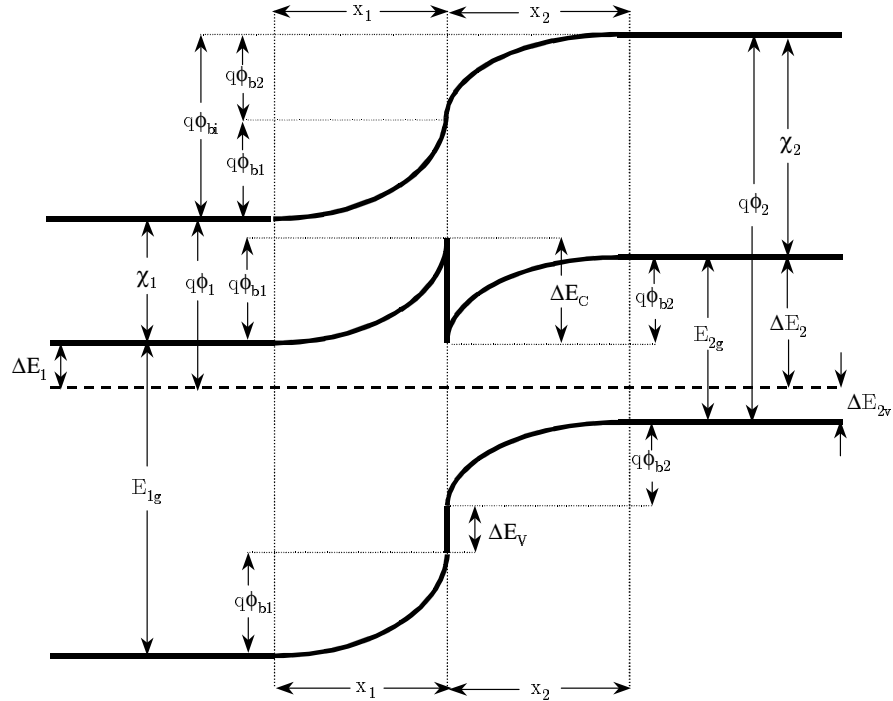|	$Al_{0.40}Ga_{0.60}As$	$GaAs$
$\chi \ [eV]$	3.63	4.07
$E_g \ [eV]$	1.92	1.42
ϵ_r	11.6	12.9
$N_C \ [cm^{-3}]$	5.0×10^{17}	4.7×10^{17}
$N_V \ [cm^{-3}]$	8.0×10^{18}	7.0×10^{18}
$N_A \ [cm^{-3}]$	—	6.0×10^{17}
$N_D \ [cm^{-3}]$	2.0×10^{17}	—

Figure 3: A N-p junction between $Al_{0.4}Ga_{0.6}As$ and $GaAs$.

$$\Delta E_g = E_{g,2} - E_{g,1} = -0.5 \ eV$$

$$\Delta E_{2,v} = \frac{k_B T}{q} ln \left(\frac{N_{V,2}}{N_{A,2}} \right) = 0.064 \ eV$$

$$\Delta E_2 = E_{g2} - \Delta E_{2,v} = 1.356 \ eV$$

$$\Delta E_1 = \frac{k_B T}{q} ln \left(\frac{N_{C,1}}{N1} \right) = 0.024 \ eV$$

$$\Delta E_c = \chi_1 - \chi_2 = -0.440 \ eV$$

$$\Delta E_v = \Delta E_c - \Delta E_g = 0.060 \ eV$$

$$q\phi_1 = \chi_1 + \Delta E_1 = 3.654 \ eV$$

$$q\phi_2 = \chi_2 + \Delta E_2 = 5.426 \ eV$$

$$q\phi_{bi} = q\phi_2 - q\phi_1 = 1.773 \ eV$$

$$x_1 = \sqrt{\frac{2N_2 \cdot \epsilon_1 \cdot \epsilon_2 \cdot q\phi_{bi}}{q \cdot N_1 (\epsilon_1 N_1 + \epsilon_2 N_2)}} = 93.508 \ nm$$

$$x_2 = \frac{N_1}{N_2} x_1 = 31.169 \ nm$$

$$q\phi_{b1} = q \left[\frac{q}{2\epsilon_1} N_1 x_1^2 \right] = 1.364 \ eV$$

$$q\phi_{b2} = q \left[\frac{q}{2\epsilon_2} N_2 x_2^2 \right] = 0.409 \ eV$$

i. How much does the conduction band spike extend above the conduction band edge in the quasi-neutral region on the p-side?
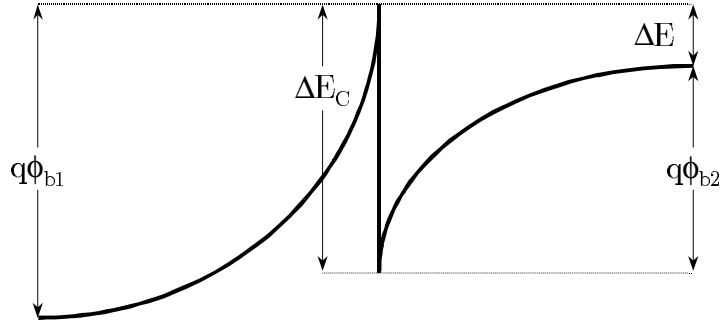

Figure 4: The conduction band spike.

$$\Delta E = \Delta E_c - q\phi_{b2} = 0.031 \ eV$$

ii. What is the applied voltage where $\Delta E = 0$?

The variables with a hat are the non-equilibrium values for the quantities that they represent. If $\Delta E = 0$, then:

$$\Delta E_c = q\hat{\phi}_{b2}$$

$$q\hat{\phi}_{b2} = q\left[\frac{q}{2\epsilon_2}N_A\hat{x}_2^2\right]$$

$$\hat{x}_2 = \sqrt{\frac{2\epsilon_2\hat{\phi}_{b2}}{qN_A}} = 32.336\ nm$$

$$\hat{x}_1 = \frac{N_A}{N_D}\hat{x}_2$$

$$q\hat{\phi}_{bi} = q\left[\frac{q}{2}\left(\frac{N_D}{\epsilon_1}\hat{x}_1^2 + \frac{N_A}{\epsilon_2}\hat{x}_2^2\right)\right] = 1.908\ eV$$

$$V_A = \phi_{bi} - \hat{\phi}_{bi} = -0.134\ Volts$$

iii. Over what distance must the junction be graded such that the spike is eliminated?

Grading the junction adds a linear function to the conduction band, as shown in Figure 5. A parabola superimposed with a line results with a shifted parabola as shown in Figure 6. The minimum distance will occur when the slope of the shifted parabola is zero, as shown in Figure 6c.

For this problem, the origin will be placed at the depletion region and all the energies the edge of the conduction band in the quasi-neutral region. The equation for E_c for $x \in [x_d - x_g, x_d]$ before grading is given by:

$$E_c(x) = q\left(\frac{q}{2\epsilon_1}N_D x^2\right) \tag{2}$$

The linear function that will be superimposed to [2] for $x \in [x_d - x_g, x_d]$ can be written as:

$$f(x) = \frac{\Delta\chi}{x_g}(x - (x_d - x_g))$$

where $\Delta\chi = \chi_2 - \chi_1 = 0.44eV$, x_g is the length of the graded region, and x_d is the depletion region length in the n-type $Al_{0.4}Ga_{0.6}As$. The conduction band edge follows the relation for $x \in [x_d - x_g, x_d]$:

$$E_c'(x) = E_c(x) - f(x)$$
$$= q\left(\frac{q}{2\epsilon_1}N_D x^2\right) - \frac{\Delta\chi}{x_g}(x - (x_d - x_g))$$

To find the minimum point,

$$\left.\frac{dE_c'}{dx}\right|_{x=x_d-x_g} = = \frac{d}{dx}\left.q\left(\frac{q}{2\epsilon_1}N_D x^2\right) - \frac{\Delta\chi}{x_g}(x - (x_d - x_g))\right|_{x=x_d-x_g} 0$$
$$= \frac{q^2}{\epsilon_1}N_D(x_d - x_g) - \frac{\Delta\chi}{x_g} = 0 \tag{3}$$

Rearranging [3]:

$$\frac{q^2}{\epsilon_1}N_D(x_d - x_g)x_g - \Delta\chi = 0$$

$$x_g^2 - x_d + \frac{\epsilon_1\Delta\chi}{q^2N_D} = 0$$

$$x_g = \frac{x_d - \sqrt{x_d^2 - 4\frac{\epsilon_1\Delta\chi}{q^2N_D}}}{2} = 19.079\ nm$$
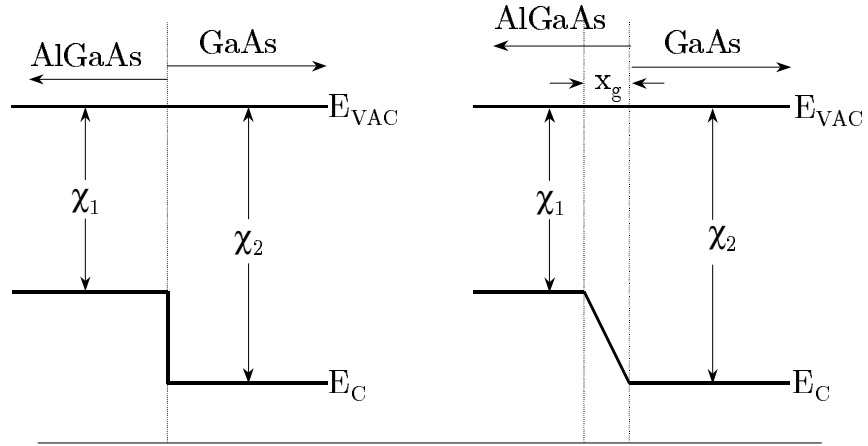
Figure 5: The vacuum energy is used as the reference, opposed to using the Fermi energy.
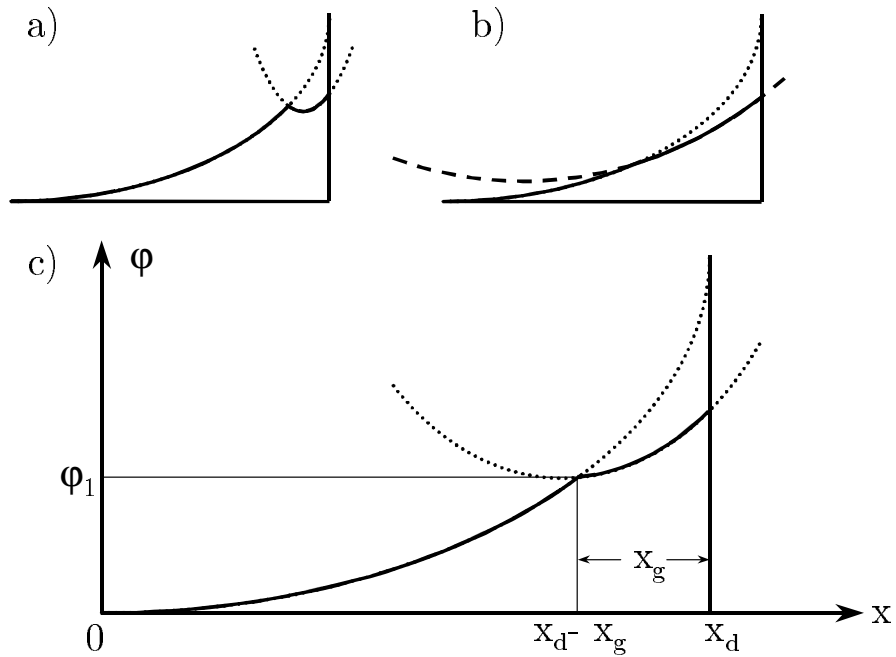

Figure 6: The result of grading the junction. The conduction band edge is used as the reference.
a) The grading length is too short. A spike forms.
b) The spike dissapears if the grading length is too long, but you are asked to find the minimum length.
c) The minimum length needed to remove the spike. Note that the slope of the conduction band is zero where the grading stops.

Problem 2.3

The density of states is given by:

$$\rho(E) = \frac{m^*}{\pi \hbar^2}$$

Part a: What is the sheet electron density for a 4 nm GaAs quantum well before the n=2 level becomes occupied?

Using [1]:

$$
\begin{aligned}
E_1(L_x = 4nm) &= 0.336\ eV \\
E_2(L_x = 4nm) &= 1.343\ eV \\
\Delta E = E_2 - E_1 &= 1.007\ eV \\
\sigma = \int \rho(E) f(E) dE &= \frac{m^*}{\pi \hbar^2} \Delta E = 7.363 \times 10^{19}\ cm^{-3} \\
D = \sigma L_x &= 2.945 \times 10^{13}\ cm^{-2}
\end{aligned}
$$

Part b: What is the sheet electron density for a 4 nm GaAs quantum well before the n=3 level becomes occupied?

$$
\begin{aligned}
E_3(L_x = 4nm) &= 3.022\ eV \\
\Delta E_{3,2} = E_3 - E_2 &= 1.679\ eV \\
\Delta E_{3,1} = E_3 - E_1 &= 2.686\ eV \\
\sigma = \int \rho(E) f(E) dE &= \rho \Delta E_{3,2} + \rho \Delta E_{3,1} = 3.191 \times 10^{20}\ cm^{-3} \\
D = \sigma L_x &= 1.276 \times 10^{14}\ cm^{-2}
\end{aligned}
$$

Part c: What is the sheet heavy hole density for a 4 nm GaAs quantum well before the n=2 level becomes occupied?

$$
\begin{aligned}
E_1(L_x = 4nm) &= 0.047eV \\
E_2(L_x = 4nm) &= 0.188eV \\
\Delta E = E_2 - E_1 &= 0.141eV \\
\sigma = \int \rho(E) f(E) dE &= \frac{m^*}{\pi \hbar^2} \Delta E = 7.363 \times 10^{19} cm^{-3} \\
D = \sigma L_x &= 2.945 \times 10^{13} cm^{-2}
\end{aligned}
$$

Problem 2.4

Part b should be solved before part a.

Part b: How long does it take to deposit one monolayer of material?

From Figure 7, a monolayer is $\frac{a}{2}$ thick. In the $[1, 0, 0]$ direction, the only difference between each gallium layer is a shift in the plane that the atoms preside in. The same is true for arsenic atoms. In GaAs, $a = 5.6533$ Å, and one monolayer is $282.67 \times 10^{-12}\ m$ thick. The growth rate is given by:

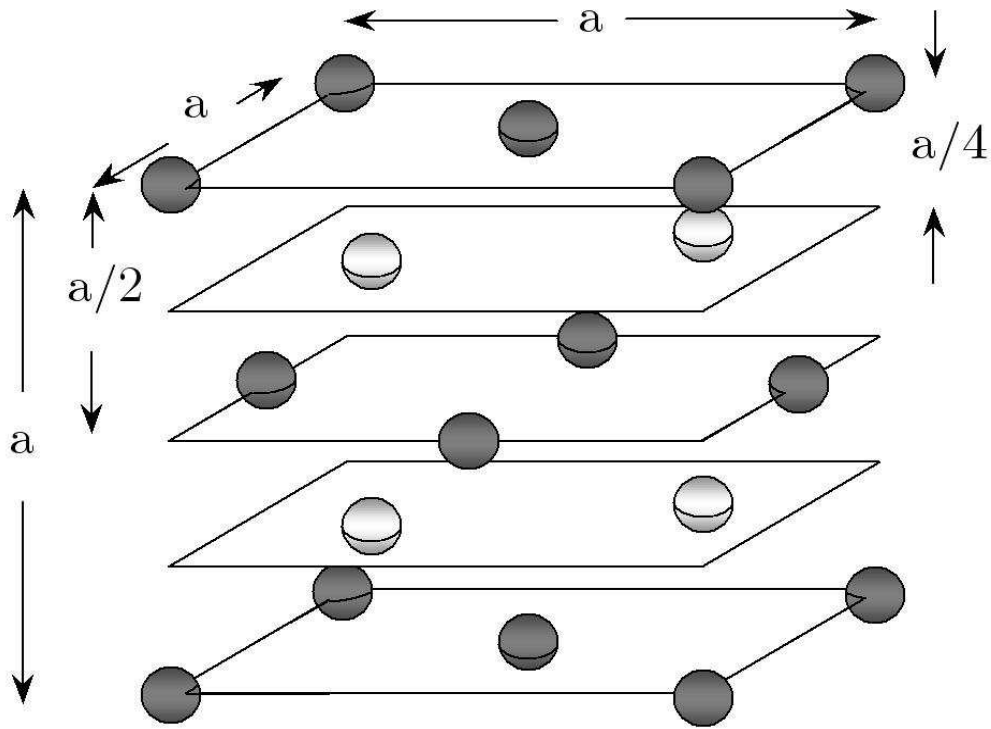Figure 7: Unit cell of a zinc-blende lattice.Note that the density of each layer is the same (2 atoms/layer).

$$
\begin{aligned}
\frac{1 \ \mu m}{1 \ hour} &= \frac{1 \times 10^{-6} \ m}{3600 \ sec} = 277.78 \times 10^{-12} \ \frac{m}{s} \\
\frac{277.78 \times 10^{-12} \ \frac{m}{s}}{282.67 \times 10^{-12} \ \frac{m}{monolayer}} &= 0.98271 \ \frac{monolayers}{sec} \cong 1 \ \frac{monolayer}{second}
\end{aligned}
$$

The growth rate is 1 monolayer per second.

Part a: What rate is must the gallium atoms must be supplied to the surface?

Each unit cell plane consists of two atoms in the area a^2. If one monolayer is provided per second, the rate (flux) is:

$$
\frac{2 \ \frac{atoms}{sec}}{a^2} = 625.79 \times 10^{12} \ cm^{-2} s^{-1}
$$

Part c: What is the thermal velocity of the gallium atom, and the distance traveled before the next monolayer is deposited for T=300K and 800K?

A gallium atom weighs $115.8 \times 10^{-27} \ kg$. The thermal energy is given by:

$$\begin{aligned} T &= \frac{k_B T}{2} = \frac{1}{2} m v^2 \\ v &= \sqrt{\frac{k_B T}{m}} \\ v\,(300\ \text{K}) &= 189.09\ \frac{m}{s} \\ v\,(800\ \text{K}) &= 308.77\ \frac{m}{s} \end{aligned}$$

Lets assume that the arsenic atoms arrive 0.5 seconds after the gallium layer is deposited. So:

$$\begin{aligned} d &= \frac{v}{t} \\ d\,(300\ \text{K}) &= 94.54\ m \\ d\,(800\ \text{K}) &= 154.38\ m \end{aligned}$$