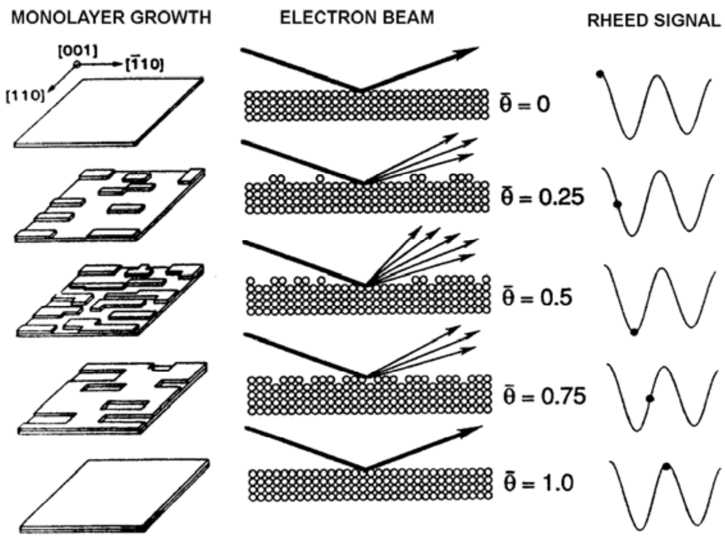
Exercise Series 1 Solutions

Wednesday, February 26th 2025

EXERCISE 1.

(a) The growth of each monolayer must pass through stages of island nucleation, growth and coalescence:



A complete monolayer reflects the beam well, giving an intense RHEED signal.
As the monolayer grows, the surface becomes rougher causing scattering → weaker RHEED signal.
Intense RHEED signal is regained on completion of the monolayer.

THEREFORE: each oscillation represents the growth of one complete monolayer.

(b) In total, there are 21 RHEED peaks from growth start to shutter closing.
These peaks occur from $t \approx 1.25$s to $t \approx 28.50$s (first peak to last peak):

21 peaks in RHEED represent the growth of 20 monolayers.

i.e., $n = 20$, $\Delta t = 28.50 - 1.25 = 27.25$

$\therefore$ growth rate $= \dfrac{n}{\Delta t}$ monolayers s^{-1}.

But the question asks for the growth rate in $\mu m\ hr^{-1}$.

$\therefore$ growth rate $= \dfrac{3600\, n x}{\Delta t}$ where x is the thickness of a GaAs (001) monolayer in μm.

The question provides $a = 5.653$ Å, but one monolayer is one Ga plane and one As plane, which is only HALF the lattice parameter.

$\therefore x = (10^{-4})\frac{a}{2}$, $\therefore$ growth rate $= \dfrac{3600(10^{-4})na}{\ldots}$

and one As plane, which is only HALF the lattice parameter.

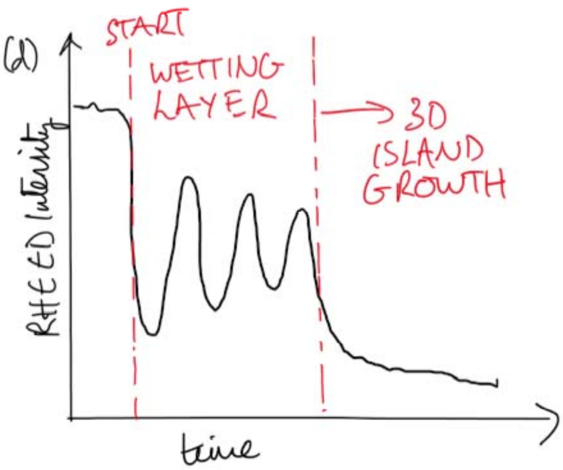
$\therefore x = (10^{-4})\frac{a}{2}$, $\therefore$ growth rate $= \frac{3600(10^{-4})na}{2\Delta t}$

$$= \frac{3600(10^{-4})(20)(5.653)}{2(27.25)} = 0.747\ \mu m\ hr^{-1}$$

(c) The peak intensity decreases over time since the growth is not actually perfectly monolayer-by-monolayer. Instead, the growth of the next monolayer will actually begin before the previous one is complete. This leads to kinetic roughening which increases over time, causing more scattering of the electron beam as growth progresses and a slow drop off in RHEED intensity over time.

For true monolayer-by-monolayer growth, see Atomic Layer Deposition (ALD).

(d)



Initially, growth in the Stranski–Krastanov regime proceeds monolayer-by-monolayer, causing the normal RHEED oscillations.

However, after the initial wetting layer, growth of large 3D islands starts in order to relax strain. This prevents specular reflection of the electron beam, causing a permanent drop in RHEED intensity.

(e) RHEED uses a high-energy electron beam to probe the surface during growth

$\Rightarrow$ high-energy electron beams require ultra-high vacuum to avoid the collision of electrons with other matter.

MOCVD is not carried out under UHV due to the input flow of reactant gases – so the use of an electron beam (and hence RHEED) is impossible.

EXERCISE 2

(a) In general form, the Schrödinger equation is: $\hat{H}\Psi = E\Psi$

where $\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$

(a) In general form, the Schrödinger equation is: $\hat{H}\Psi = E\Psi$

where $\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$

kinetic potential

For this case, we only care about the z dimension, and $V(z) = 0$ within the well.

$$\therefore \boxed{-\frac{\hbar^2}{2m_e^*}\frac{d^2\chi_n}{dz^2} = \mathcal{E}_n \chi_n}$$

The relevant boundary conditions arise from the requirement of continuity in χ_n at the points where the quantum well meets the barrier, i.e, $z=0$ and $z=L$.

Since $V=\infty$ in the barrier, by necessity $\chi_n = 0$ in the barrier. Hence for continuity to hold:

$$\boxed{\chi_n(z=0) = 0 \quad \text{and} \quad \chi_n(z=L) = 0}$$

These are the relevant boundary conditions.

(b) $\chi_n = A\sin(k_n z) + B\cos(k_n z)$

$$\therefore \frac{d^2\chi_n}{dz^2} = -k_n^2\left(A\sin(k_n z) + B\cos(k_n z)\right) = -k_n^2\chi_n$$

From part (a): $-\frac{\hbar^2}{2m_e^*}\frac{d^2\chi_n}{dz^2} = \mathcal{E}_n\chi_n \Rightarrow -\frac{\hbar^2}{2m_e^*}(-k_n^2\chi_n) = \mathcal{E}_n\chi_n$

$$\therefore \frac{\hbar^2 k_n^2}{2m_e^*}\cancel{\chi_n} = \mathcal{E}_n\cancel{\chi_n} \quad , \quad \boxed{\mathcal{E}_n = \frac{\hbar^2 k_n^2}{2m_e^*}}$$

(c) $\chi_n(z=0) = 0$ ① , $\chi_n(z=L) = 0$ ②

① $\therefore A\sin(0) + B\cos(0) = 0 \Rightarrow B = 0$

② $\therefore A\sin(k_n L) = 0$, $\therefore k_n L = n\pi \Rightarrow k_n = \frac{n\pi}{L}$ where n is any positive integer.

As such we have shown k_n is quantized → only certain values of k allow for the boundary conditions to be met.

$$\therefore \chi_n = A\sin\left(\frac{n\pi z}{L}\right), \text{ and } \mathcal{E}_n = \frac{\hbar^2 k_n^2}{2m_e^*} = \boxed{\frac{\hbar^2\pi^2 n^2}{2m_e^* L^2}}$$

To normalise the wavefunction, we must ensure $\int_0^L |\chi_n|^2\, dz = 1$.

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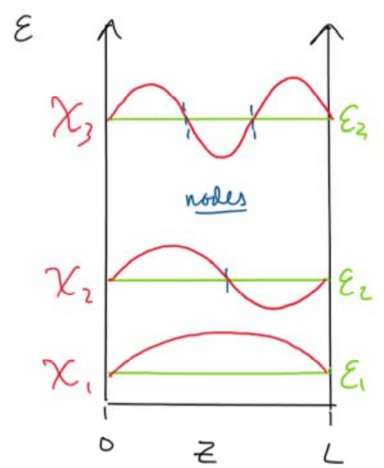
This is because $|\chi_n|^2 dz$ represents the probability that the electron will be in the interval $dz \Rightarrow$ since the electron must be somewhere in the quantum well (as it can't be in the barriers) the probability of finding it in the well must $= 1$.

$$\int_0^L |\chi_n|^2 dz = \int_0^L A^2 \sin^2\left(\frac{n\pi z}{L}\right) dz = \frac{A^2}{2}\int_0^L 1 - \cos\left(\frac{2n\pi z}{L}\right) dz$$

$$= \frac{A^2}{2}\left[z - \frac{L}{2n\pi}\sin\left(\frac{2n\pi z}{L}\right)\right]_0^L = \frac{A^2}{2}(L-0) = \frac{A^2 L}{2}$$

$$\therefore \frac{A^2 L}{2} = 1, \quad A = \sqrt{\frac{2}{L}} \qquad \boxed{\therefore \chi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right)}$$

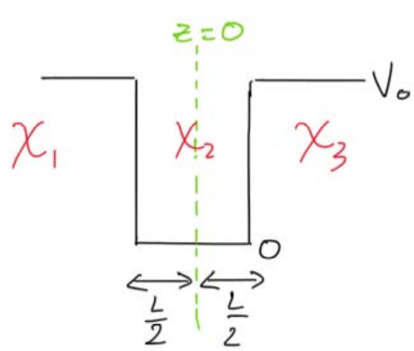
General comments: • n cannot be zero, since this corresponds to $\chi = 0$, i.e there is no electron. Clearly this isn't of interest.



• We see that ε_1 (the ground state energy) has an energy greater than zero. This "zero point energy" is linked to Heisenberg's uncertainty principle $\Delta p \Delta z \geq \hbar/2$. If the ground state energy were to equal zero, this would imply an electron momentum of zero and hence $\Delta p = 0$. In order for the uncertainty principle to be at all satisfied, Δz would have to be ∞ - yet we know the electron is in the well with finite width L, so actually $\Delta z = L$. Hence the ground state energy must be greater than zero to satisfy Heisenberg's uncertainty principle.
We can see from our solutions for ε_n that $\varepsilon_1 \to 0$ as $L \to \infty$, so as always we restore classical behaviour for macroscopic dimensions (in everyday life, objects placed in boxes do not have to have non-zero kinetic energy!)

• Higher energy states have points where $\chi_n = 0$ (nodes) - there is then zero probability of finding the electron at this point in the well for that certain state. This is a purely quantum mechanical effect and has no classical analogue.

In order to avoid any confusion about the finite-barrier square quantum well, I will go through the FULL derivation here. I will mark when the direct answer to part (d) actually begins.



$$V(z) = \begin{cases} V_0 & \text{for } z < -L/2 \\ 0 & \text{for } -L/2 \leq z \leq L/2 \\ V_0 & \text{for } z > L/2 \end{cases}$$

N.B. the z origin is now in the centre of the quantum well.

Since the barrier potential is now finite, the electron can exist in the barrier, so the wavefunction will no longer be zero here.
Due to the piecewise potential, we define the wavefunction:

$\overset{\longleftrightarrow}{\frac{L}{2}} \;|\; \overset{\longleftrightarrow}{\frac{L}{2}}$

here.

Due to the piecewise potential, we define the wavefunction:

$$\chi = \begin{cases} \chi_1 & \text{for } z < -L/2 \quad \text{OUTSIDE} \\ \chi_2 & \text{for } -L/2 \leq z \leq L/2 \quad \text{INSIDE} \\ \chi_3 & \text{for } z > L/2 \quad \text{OUTSIDE} \end{cases}$$

Crucially, the barrier material is likely to be different from the well material, so the electron effective masses will be different: m_A^* in the well, and m_B^* in the barrier.

As usual, Schrödinger: $-\frac{\hbar^2}{2m}\frac{d^2\chi}{dz^2} + V(z)\chi = \mathcal{E}\chi$

Inside the well

$V(z)=0$, $-\frac{\hbar^2}{2m_A^*}\frac{d^2\chi_2}{dz^2} = \mathcal{E}\chi_2 \Rightarrow$ this is identical to the initial case for the infinite quantum well, so we know solutions will be of the form:

$\chi_2 = A\sin(kz) + B\cos(kz)$, which will give $\mathcal{E} = \frac{\hbar^2 k^2}{2m_A^*}$, $k = \frac{\sqrt{2m_A^*\mathcal{E}}}{\hbar}$

Outside the box

First considering χ_1 in region $z < -L/2$:

$V(z) = V_0$, $-\frac{\hbar^2}{2m_B^*}\frac{d^2\chi_1}{dz^2} + V_0\chi_1 = \mathcal{E}\chi_1$, $\therefore -\frac{\hbar^2}{2m_B^*}\frac{d^2\chi_1}{dz^2} = (\mathcal{E}-V_0)\chi_1$

In this case, the relevant general solution is $\chi_1 = Ce^{-\kappa z} + De^{\kappa z}$, which when put into the above Schrödinger equation gives:

$-\frac{\hbar^2\kappa^2}{2m_B^*}\cancel{\chi_1} = (\mathcal{E}-V_0)\cancel{\chi_1}$ $\quad\therefore\quad \kappa = \frac{\sqrt{2m_B^*(V_0-\mathcal{E})}}{\hbar} \rightarrow$ this is only valid for $\mathcal{E} \leq V_0$, which shows we are only considering BOUND states.

Similarly, for χ_3 we get the same results, with $\chi_3 = Ee^{-\kappa z} + Fe^{\kappa z}$.

We can already apply some boundary conditions: in order for wavefunctions to be physically reasonable:

$\chi_1(z=-\infty) = 0$ ①, $\chi_3(z=+\infty) = 0$ ② $\rightarrow$ we don't expect to find bound electrons infinitely far from the well!

These conditions lead to:

$C=0$, $F=0$. So: $\chi_1 = De^{\kappa z}$, $\chi_3 = Ee^{-\kappa z}$

Applying full boundary conditions

So far, we have:

$$\chi = \begin{cases} De^{\kappa z} & z < -L/2 \\ A\sin(kx) + B\cos(kx) & -L/2 \leq z \leq L/2 \\ Ee^{-\kappa z} & z > L/2 \end{cases}$$

with $k = \frac{\sqrt{2m_A^*\mathcal{E}}}{\hbar}$, and $\kappa = \frac{\sqrt{2m_B^*(V_0-\mathcal{E})}}{\hbar}$

$C = D$

$H = E$

$$\mathcal{E} e^{-Kz} \qquad z > L/2 \qquad\qquad C = D$$

with $k = \dfrac{\sqrt{2 m_A^* \varepsilon}}{\hbar}$, and $K = \dfrac{\sqrt{2 m_B^* (V_0 - \varepsilon)}}{\hbar}$ $\qquad H = \mathcal{E}$

Now, as for the infinite well, χ must be continuous. In addition, an extra condition arises from the fact we are dealing with finite potentials: the particle current of χ must also be continuous. Of course, the region where we must check this is at the boundaries, so the final conditions are:

$$\chi_1(z=-L/2) = \chi_2(z=-L/2) \ ③ \ , \ \chi_2(z=L/2) = \chi_3(z=L/2) \ ④$$

$$\frac{1}{m_B^*}\frac{d\chi_1}{dz}\bigg|_{z=-L/2} = \frac{1}{m_A^*}\frac{d\chi_2}{dz}\bigg|_{z=-\frac{L}{2}} \ ⑤, \quad \frac{1}{m_A^*}\frac{d\chi_2}{dz}\bigg|_{z=L/2} = \frac{1}{m_B^*}\frac{d\chi_3}{dz}\bigg|_{z=\frac{L}{2}} \ ⑥$$

These conditions have two solutions - an even case and an odd case.

For the even case, $A = 0$ and $D = \mathcal{E}$, for the odd case $B = 0$ and $D = -\mathcal{E}$.

i.e,

even

$$\chi = \begin{cases} \mathcal{E} e^{Kz} & z < -L/2 \\ B\cos(kz) & -L/2 \le z \le L/2 \\ \mathcal{E} e^{-Kz} & z > L/2 \end{cases}$$

odd

$$\chi = \begin{cases} -\mathcal{E} e^{Kz} & z < -L/2 \\ A\sin(kz) & -L/2 \le z \le L/2 \\ \mathcal{E} e^{-Kz} & z > L/2 \end{cases}$$

Applying the boundary conditions to these solutions:

even ③ $\mathcal{E} e^{-KL/2} = B\cos\left(-\frac{kL}{2}\right) = B\cos\left(\frac{kL}{2}\right)$ $\Rightarrow$ condition ④ gives the same.

⑤ $\frac{K\mathcal{E}}{m_B^*} e^{-KL/2} = \frac{kB}{m_A^*}\sin\left(-\frac{kL}{2}\right) = \frac{k}{m_A^*}B\sin\left(\frac{kL}{2}\right)$ $\Rightarrow$ " ⑥ " " "

Taking the ratio of these equations, we find: $\dfrac{K}{m_B^*} = \dfrac{k}{m_A^*}\tan\left(\dfrac{kL}{2}\right)$

odd ③ $-\mathcal{E} e^{-KL/2} = A\sin\left(-\frac{kL}{2}\right) = -A\sin\left(\frac{kL}{2}\right)$ $\Rightarrow$ same for ④

⑤ $-\frac{K}{m_B^*}\mathcal{E} e^{-KL/2} = \frac{kA}{m_A^*}\cos\left(-\frac{kL}{2}\right) = \frac{kA}{m_A^*}\cos\left(\frac{kL}{2}\right)$ $\Rightarrow$ same for ⑥

Taking the ratio again: $\dfrac{K}{m_B^*} = -\dfrac{k}{m_A^*}\cot\left(\dfrac{kL}{2}\right)$

- - - - - - - - - - - - - - - - POINT WHERE (d) REALLY STARTS

We have now set up everything we need to find the expression for N, the number of bound states.

Assuming $m_A^* \approx m_B^* = m_e^*$:

$$K = k\tan\left(\frac{kL}{2}\right) \ ⑦ \quad , \quad K = -k\cot\left(\frac{kL}{2}\right) \ ⑧$$

$$K = k\tan\left(\frac{kL}{2}\right) \quad ⑦ \qquad , \qquad K = -k\cot\left(\frac{kL}{2}\right) \quad ⑧$$

$$\underbrace{\text{where} \quad K = \frac{\sqrt{2m_e^*(V_0 - \mathcal{E})}}{\hbar} \quad , \quad k = \frac{\sqrt{2m_e^*\mathcal{E}}}{\hbar}}$$

$$\therefore \quad K^2 = \frac{2m_e^* V_0}{\hbar^2} - \frac{2m_e^*\mathcal{E}}{\hbar^2} = \frac{2m_e^* V_0}{\hbar^2} - k^2 \quad ⑨$$

Making the substitution $u = \frac{KL}{2}$, $v = \frac{kL}{2}$:

⑦: $u = v\tan v$ ⑧: $u = -v\cot v$

⑨: $\frac{4u^2}{L^2} = \frac{2m_e^* V_0}{\hbar^2} - \frac{4v^2}{L^2}$, $\therefore u^2 = \frac{m_e^* V_0 L^2}{2\hbar^2} - v^2 = u_0^2 - v^2$

where $u_0 = \sqrt{\frac{m_e^* V_0 L^2}{2\hbar^2}}$

Combining these substituted equations:

$$u = \boxed{\sqrt{u_0^2 - v^2} = \begin{cases} v\tan v & \rightarrow \text{even states} \\ -v\cot v & \rightarrow \text{odd states} \end{cases}}$$

This condition can be PLOTTED: u vs. v.

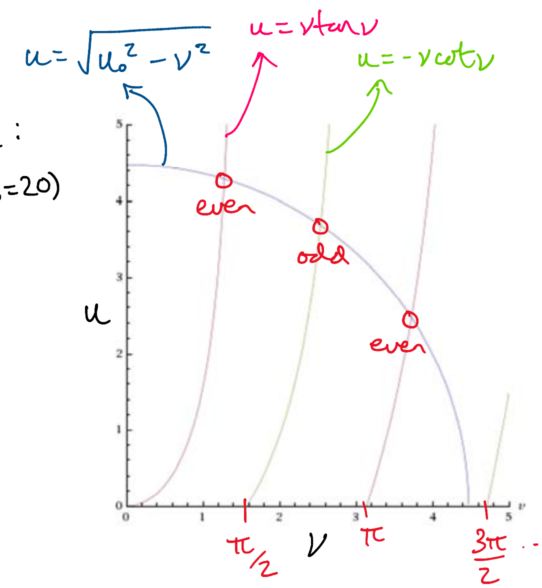
$u = \sqrt{u_0^2 - v^2}$ is a circle, radius u_0 and centre $u = 0$, $v = 0$.

$u = v\tan v$ and $u = -v\cot v$ are "periodic" with period $= \pi$, and staggered relative to each other by $\frac{\pi}{2}$.

Crucially, the boundary conditions apply separately to the even and odd states. So the condition $u = v\tan v$ does not have to be satisfied at the same time as $u = -v\cot v$. Of course, this would be impossible since $v\tan v = -v\cot v$ has no solutions.

So, we must consider $\sqrt{u_0^2 - v^2} = v\tan v$ separately from $\sqrt{u_0^2 - v^2} = -v\cot v$. Each solution to the first equation represents a bound even state, for the second there is a bound odd state.

e.g.:
(for $u_0^2 = 20$)



We are only interested in positive K and k, hence we only inspect for positive u and v as they are proportional to K and k.

Now, the intersections on this plot give the values of u and v (and hence K and k) for which the boundary conditions are valid - i.e, each intersection represents a BOUND STATE.

For example, in the left plot for $u_0^2 = 20$, we have three bound states.

We can generalise this graphical interpretation: because in the positive quadrant $v\tan v$ and $-v\cot v$ taken together stretch from 0 to ∞ every $\pi/2$ in v, we can write that each intersection value v_i :

write that each intersection value ν_i:

$$\frac{\pi}{2}(i-1) \le \nu_i < \frac{\pi}{2} i \Rightarrow$$ As such, the total number of bound states is found by dividing the radius of the circle, u_0, by the interval required for each ν_i value.

$$n = u_0 \div \frac{\pi}{2} = \frac{2u_0}{\pi}$$

But, we must remember that the circle only has to enter a new $\pi/2$ interval in order for there to be another new ν_i intersection (since $\nu\tan\nu$ and $-\nu\cot\nu$ start from zero at the beginning of each interval). As such, to obtain the actual number of bound states N, we must round n up:

$$N = \lceil n \rceil = \left\lceil \frac{2u_0}{\pi} \right\rceil = \left\lceil \frac{2}{\pi}\left(\frac{m_e^* V_0 L^2}{2\hbar^2}\right)^{1/2} \right\rceil$$

$$\therefore \boxed{N = \left\lceil \left(\frac{2 m_e^* V_0 L^2}{\pi^2 \hbar^2}\right)^{1/2} \right\rceil}$$

Comments:
- Since we have a ceiling function, we have shown that no matter the barrier height (V_0) / width (L) / effective mass (m^*_e), there is always at least one bound state in the quantum well.
- Increasing the barrier height leads to more bound states - as expected for a deeper potential, more states can be accommodated before $\varepsilon > V_0$.
- Increasing the well width also leads to more bound states - a wider well means smaller energy spacing between the energy levels, so more states can again be accommodated before $\varepsilon > V_0$.
- Greater effective mass has a similar effect to increasing the well width.

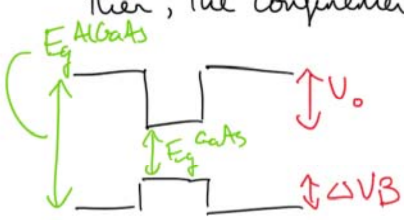
(e) First, we need to find $E_g^{Al_{0.3}Ga_{0.7}As}$; using the expression given in the question:

$$E_g^{Al_{0.3}Ga_{0.7}As} = (0.3)(3.13) + (0.7)(1.52) - (0.3)(0.7)[-0.127 + 1.31(0.3)]$$
$$= 1.95 \text{ eV}$$

Then, using the general rule for III-V compounds sharing the same anion (Lecture 2 slide 28) we can find the valence band offset of GaAs to $Al_{0.3}Ga_{0.7}As$ ΔVB:

$$\Delta VB \approx 0.3\Delta E_g = 0.3\,(E_g^{Al_{0.3}Ga_{0.7}As} - E_g^{GaAs})$$

Then, the confinement potential in the conduction band is given by:



$$V_0 = E_g^{Al_{0.3}Ga_{0.7}As} - E_g^{GaAs} - \Delta VB$$
$$= 0.7(E_g^{Al_{0.3}Ga_{0.7}As} - E_g^{GaAs})$$
$$= 0.7(1.95 - 1.52) = 0.301 \text{ eV}$$

Here, using our expression for N and knowing $m_e^* = 0.067\, m_0$ and $L = 12$ nm:

$$N = \left\lceil \left(\frac{2(0.067 \times 9.11 \times 10^{-31})(0.301 \times 1.602 \times 10^{-19})(12 \times 10^{-9})^2}{\pi^2 (1.055 \times 10^{-34})^2} \right)^{\frac{1}{2}} \right\rceil$$

$$= \lceil 2.78 \rceil = 3 \qquad \therefore \; N = 3$$

It is worth noting that pure AlAs is an indirect semiconductor. This affects AlGaAs too: AlGaAs with an AlAs fraction higher than $\approx 40\%$ is also indirect. This means AlGaAs is rarely used with AlAs $> 40\%$ - for this question, we are below the transition point.