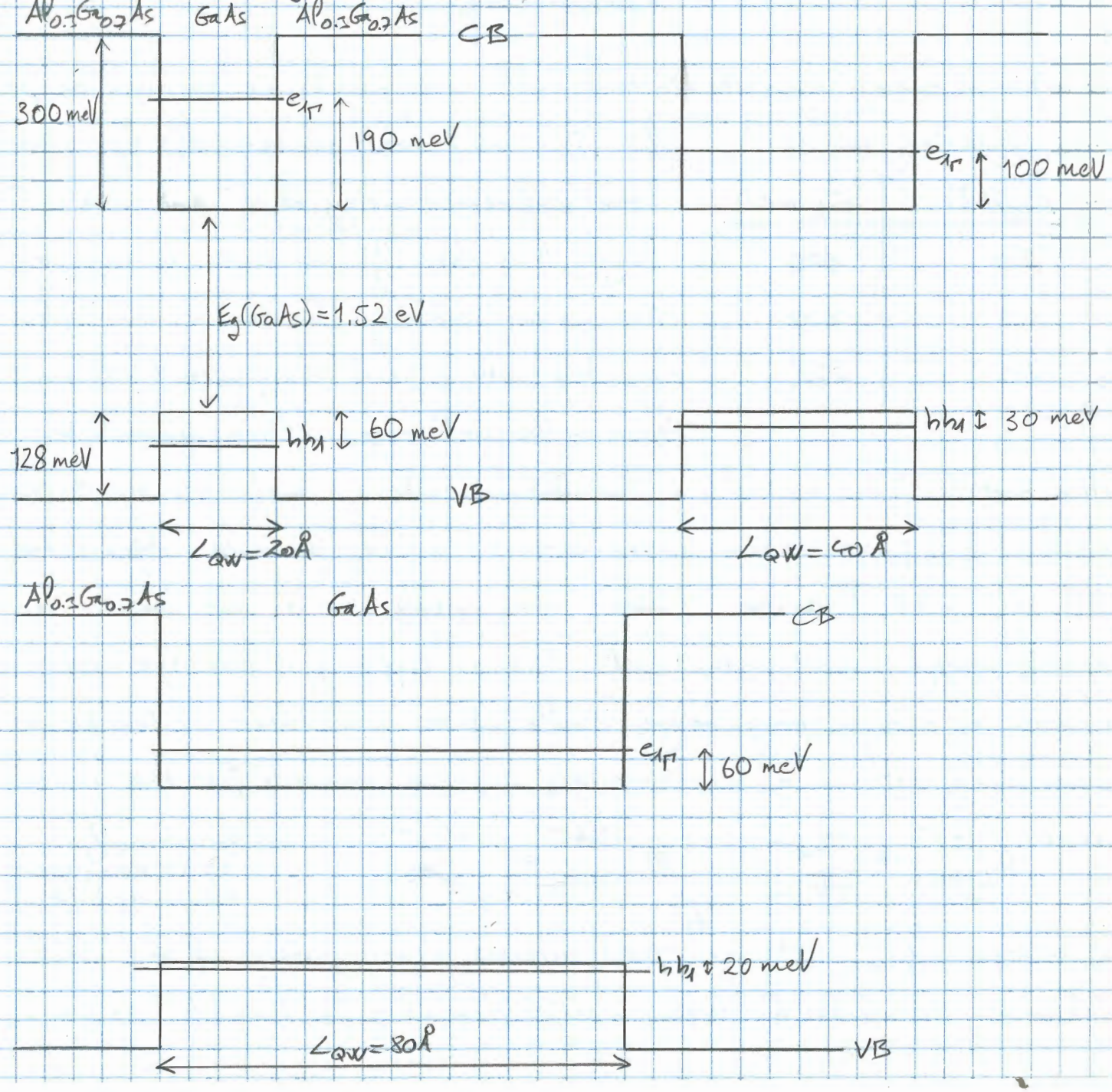
Series - Electronic and optical semiconductor devices

Series 6 - Optical properties of GaAs/AlGaAs quantum wells

1 - A) The thinner the well of interest, the larger the confinement energy. The valence band offset between the well material and the barrier material is deduced from the so-called common-anion rule which sets that:

$\Delta V = 0.3 \times (E_g(Al_{0.3}Ga_{0.7}As) - E_g(GaAs)) = 128$ meV and consequently the conduction band offset is such that: $\Delta C = 0.7 (E_g(Al_{0.3}Ga_{0.7}As) - E_g(GaAs)) = 300$ meV

As a result for type I heterostructures electrons are more confined than holes.



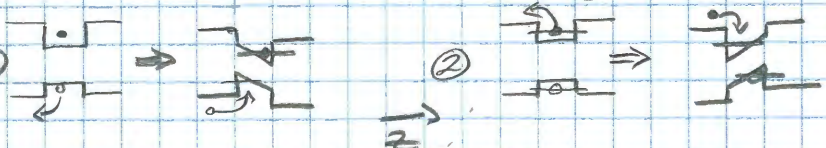
B) It is seen that for Al concentrations $x_{Al} \geq 0.42$, the AlGaAs alloy becomes an indirect band gap semiconductor as the minimum of the band gap does not lie anymore at the Γ point which corresponds to the center of the 1st Brillouin zone (BZ). Instead it occurs at the X point ([100] direction for zincblende crystals such as arsenide compounds). In fact, this is the minimum of the CB which is affected by the x_{Al} increase as $dE_{\Gamma c}/dx_{Al} \gg dE_{Xc}/dx_{Al}$

C) ⇒ See part (e)

D) The evolution of the PL integrated intensity with temperature is described by an Arrhenius law $I_{PL}(T) = \frac{I_0}{1 + A\exp(-E_A/k_B T)}$

The activation energy associated to each well corresponds to the thermal escape energy of exitons out of the wells. For the thinnest quantum wells for which the confinement energy of e^- and holes is larger, it is easier for an exciton to escape. This can be intuitively understood as the levels associated with e^- and heavy holes (HH) are closer to the well edges. It is essential to notice that this is the exciton (i.e. the electron-hole pair bound via the Coulomb interaction) and not only one of the carriers (namely the hole which is less confined) which will escape. Indeed, experimentally we do not observe an excess of charged carriers in the wells. Moreover supposing it were the case, the excess of one of the charges would induce a curvature of the bands which would act as a supplementary attractive potential for the "ionized" carrier.

L_{QW} (Å)	E_A (meV)
20	100
40	220
80	270



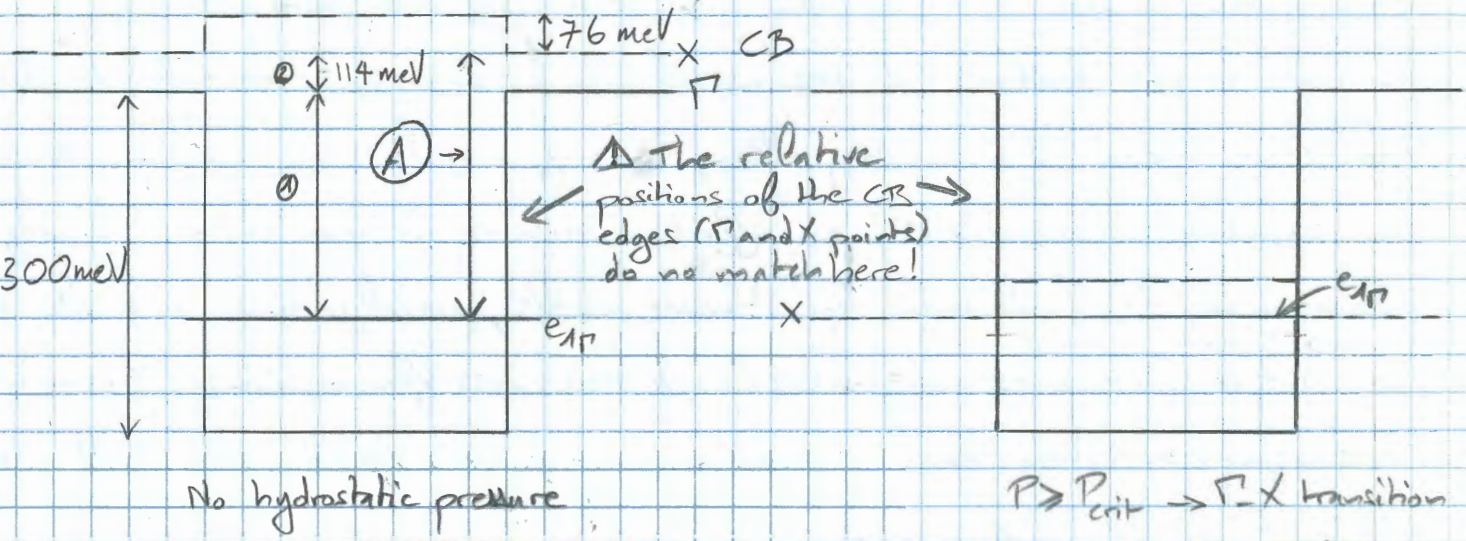
↳ formation of a dipole along the growth axis (z).

The decrease of $I_{PL}(T)$ when T(K) increases is a signature of the weaker confinement of excitons due to the increased probability for the latter to be

thermally excited out of the wells.

E) The disappearance of PL peaks at certain critical pressures can be qualitatively explained as follows: the type I PL energy increases under pressure essentially like the increase of the direct band gap of the bulk material forming the well. At a given pressure, which will depend on the well thickness L_{QW}, the fundamental state of the confined electron at the Γ point, $e_{1\Gamma}$, will cross the conduction X band edge of the barrier material. e^- will thus escape in the barrier which induces a strong decrease, and even a complete (disappearance (quenching) of the type I PL; due to a greatly decreased overlap of the e^- and hh wavefunctions (the latter remains trapped in the QW).

Physical parameters	GaAs	$Al_{0.3}Ga_{0.7}As$
E_g^Γ (meV)	1519	1947
E_g^X (meV)	2010	2061
ΔE_g (meV)	491	114
dE_g^Γ/dP (meV/GPa)	106	105
dE_g^X/dP (meV/GPa)	-13.4	-14.4



No hydrostatic pressure

$P > P_{crit}$ → Γ-X transition for the minima of the e^- level confined in the CB

Valence band structure is UNCHANGED from part (a), since the valence band maximum is always at the Γ point. (ΔV is always calculated using E_g^Γ).

When the hydrostatic pressure increases, $E_g^\Gamma \nearrow$ and $E_g^X \searrow$ so that beyond a certain pressure which will depend on the well thickness we get a crossover from a type I QW to a structure which is not radiatively active

Illustration in the case of the 20Å thick QW

For a nought applied pressure, we wish to calculate the energy difference Ⓐ = ① + ② (cf. previous figure): $Ⓐ = (\Delta C^\Gamma - e_{1\Gamma}) + (E^X_{gAlGaAs} - E^\Gamma_{gAlGaAs})$ $= 225$ meV with $\Delta C^\Gamma = 0.7 (E^\Gamma_{gAlGaAs} - E^\Gamma_{gGaAs})$

The critical pressure, P_{crit}, corresponding to the ΓX crossover is found on the figure at the intersection between the continuous and the dashed lines, which occurs at $P^{exp}_{crit} \simeq 1.75$ GPa for the 20Å thick wells.

The pressure which is required to fill this energy gap $e_{1X} - e_{1\Gamma}(0)$ will then write: $P^{th}_{crit} \frac{dE_g^\Gamma}{dP} - P^{th}_{crit} \frac{dE^X}{dP} = e - e_\Gamma(0)$

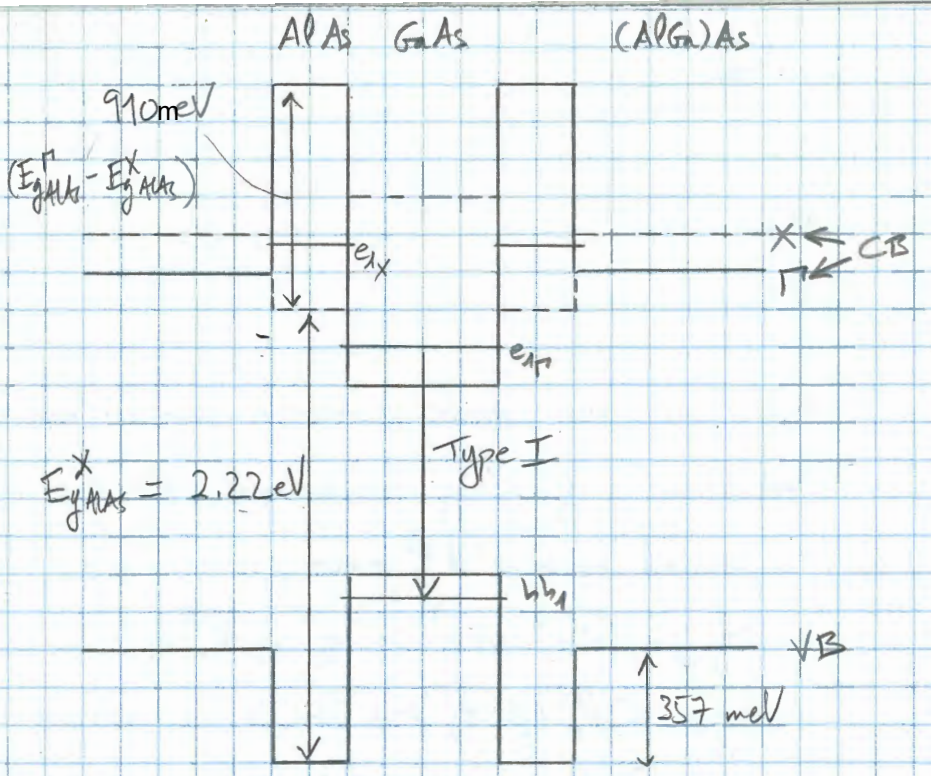
It leads to $P^{th}_{crit} = \frac{225}{(105 + 14.4)} \sim 1.88$ GPa $\Rightarrow P^{th}_{crit} \simeq P^{exp}_{crit}$

$L_{QW} = 40$Å, $P^{exp}_{crit} \sim 2.42$ GPa, $P^{th}_{crit} \sim 2.64$ GPa

$L_{QW} = 80$Å, $P^{exp}_{crit} \sim 2.95$ GPa, $P^{th}_{crit} \sim 2.97$ GPa

The increase of the PL linewidth with decreasing well thickness L_{QW} is ascribed to the leakage of the wavefunctions into the barriers. As the latter are made of a ternary alloy, wavefunctions will become sensitive to composition fluctuations, an effect which is not seen with a binary compound. In addition for thinner wells, wavefunctions will also be sensitive to the interface roughness (well thickness fluctuations...) which is less important when the wavefunctions do no "feel" the well edges...

2Ⓐ) Hereafter we will simply consider the case of a single well in absence of any hydrostatic pressure:

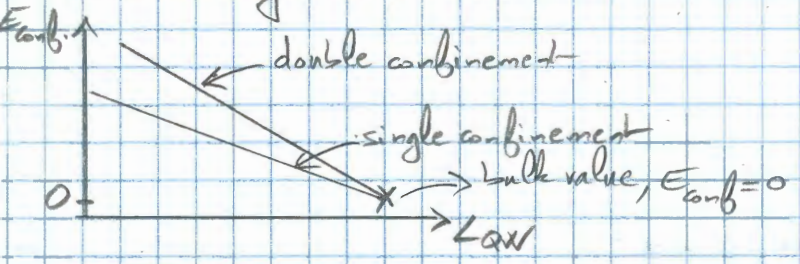


Structure in GaAs and $Al_{0.3}Ga_{0.7}As$ is unchanged from (e)

ΔV between AlGaAs and AlAs

$\Delta V^{\Gamma} = 0.3(3.13 - 1.95) = 357meV$

The AlAs monolayer having a larger band gap energy, the confinement potential of carriers is increased. Consequently, confinement energies will increase with respect to the single well case.

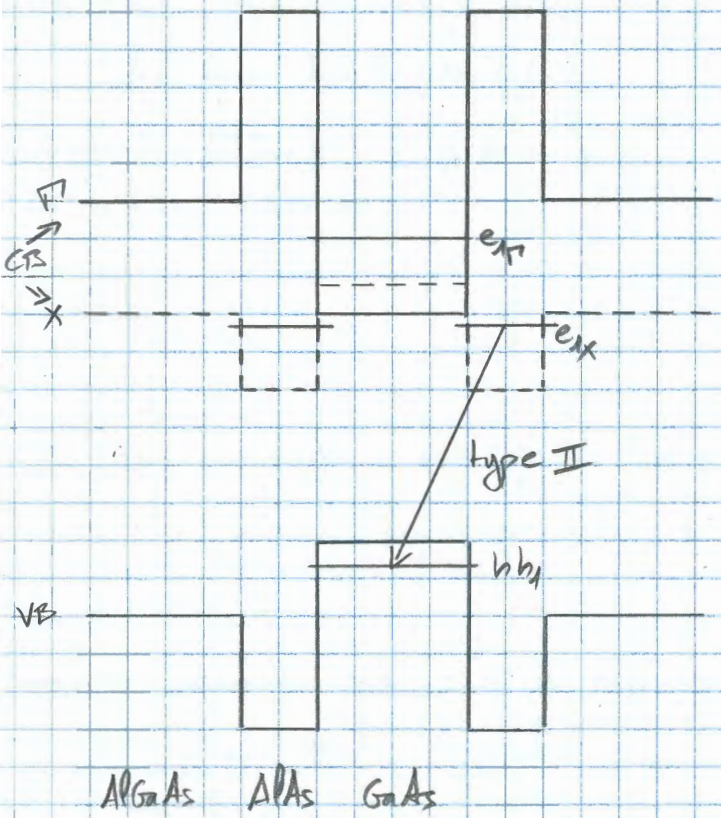


In fact, variations are not linear as they vary like $1/L^2 \Rightarrow E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}$ infinite barrier case!

B) First, the type I PL energy increases. Then beyond a certain pressure which depends once again on L_{QW} (but the values differ from the previous geometry) a decrease of the PL energy is observed which is accompanied by a drop in PL intensity. This behavior illustrates a crossover from a type I toward a type II heterostructure. The new optical transitions involve heavy holes confined in the GaAs well and e^- confined in the AlAs ML. It results from the Γ-X transition which originated from the opposite behaviors of Γ and X points under hydrostatic pressure: $\alpha_\Gamma = \frac{dE_g^{\Gamma}}{dP} > 0$ and $\alpha_X = \frac{dE_g^{X}}{dP} < 0$.

The variation of energies exhibits a linear dependence on the exerted hydrostatic pressure P: $E(P) = E(0) + \alpha P$

L_{QW} (Å)	a_Γ (meV/GPa)	a_X (meV/GPa)
20	92	-19.2
40	97	-21.2
80	102	-22.2



Note that the optical matrix element for type II transitions is given by perturbation theory expanded to the 1st order:

$$M_{CV} = (\langle \varphi_c^X | V | \varphi_c^\Gamma \rangle \langle \varphi_c^\Gamma | p | \varphi_V^\Gamma \rangle)/(E_\Gamma - E_X)$$

where $\langle \varphi_c^\Gamma | p | \varphi_V^\Gamma \rangle$ is the direct optical matrix element and $\langle \varphi_c^X | V | \varphi_c^\Gamma \rangle$ is the Γ-X mixing matrix element.

From previous figured, PL transition energid are:

$E_{PL} = E_g(GaAs) + E_e^\Gamma + E_{hh} - E_{R_y}^\Gamma - E_{loc}^\Gamma$ for a type I structure

and $E_{PL} = E_g(AlAs) - \Delta E_V + E_e^X + E_{hh} - E_{R_y}^X - E_{loc}^X$ for a type II structure.

E_{R_y} and E_{loc} stand for the exciton binding energy and the localisation energy originating from the non perfect structure of the samples, respectively.

ΔE_V is the VB offset between GaAs and AlAs.

For the three wells, when they are in the type II regime, the energy E_e^X is the same so that the PL energy difference directly illustrates the change in the hole confinement energy (when neglecting both $E_{R_y}^X$ and $E_{loc}^X \ll E_{hh}$). Then, E_e^X can be determined from E_{PL} (type II).

→ calculate confinement energies in a finite well (3)

A powerful and simple method to implement deals with the formalism of the envelope function (cf. lecture).

Further reading

M. Leroux et al., Phys. Rev. B 45, 11846 (1992)