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Interface-related band-bending effects on intersubband transitions in doped GaAs/$Al_xGa_{1-x}As$ single quantum wells

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Abstract. We show that band-bending corrections related to the existence of nonabrupt interfaces can change considerably the electron intersubband transitions in modulation-doped GaAs/$Al_xGa_{1-x}As$ single quantum wells. In our calculations, the position-dependent electron effective mass in the interface regions is taken into account, and the Poisson and Schrödinger equations for the single quantum wells are solved self-consistently. When the doping density in the barriers is 3×10^{18} cm^{-3}, we obtain that the first electron intersubband transition energy in a 100 Å single GaAs/$Al_{0.3}Ga_{0.7}As$ quantum well with nonabrupt interface widths of only 12 Å is 16 meV higher than the one calculated for a similarly doped abrupt well.

The understanding of the properties of GaAs/$Al_xGa_{1-x}As$ modulation-doped quantum wells (MDQWs) is important for the improvement of devices like infrared photodetectors [1]. Their design has always been implemented within the sharp-interface picture, where the existence of nonabrupt interfaces is disregarded. In this approach, the MDQW width, the aluminium molar content of the $Al_xGa_{1-x}As$ alloy (which determines the MDQW depth), and the doping density (generally Si or Be at concentrations of the order of 10^{18} cm^{-3}) are the relevant parameters in the modelling. However, an agreement not better than 5 meV between measurements and the theoretical calculations [2, 3] of the subband energy separation in 59 Å GaAs/$Al_xGa_{1-x}As$ MDQWs was obtained, for example. On the other hand, Fishman [4] and Ramsteiner *et al* [5] showed the existence of a reduction of the order of 10 meV in the first intersubband transition energy in GaAs/$Al_xGa_{1-x}As$ MDQWs for doping densities as high as 5×10^{18} cm^{-3}.

In fact, the interfaces in GaAs/$Al_xGa_{1-x}As$ MDQWs are not sharp. Using scanning tunnelling microscopy, Johnson *et al* [6] and Albrektsen *et al* [7] were able to show with atomic resolution images that p-doped ($(2–3) \times 10^{18}$ cm^{-3}) GaAs/$Al_xGa_{1-x}As$ multilayers in MDQWs presented interfacial transition regions that extended over one to two unit cells, in the best cases. As a consequence of the existence of nonabrupt interfaces in GaAs/$Al_xGa_{1-x}As$ MDQWs, the overall charge density changes in the doped barriers, producing a graded interface-related decrease in the degree of band bending inside the wells. Consequently, calculations performed within the sharp-interface picture should overestimate the carrier bound energies in MDQWs, a fact that generally was not considered, up to now, as an argument in attempting to achieve a better understanding of the doping density dependence of the intersubband transitions in GaAs/$Al_xGa_{1-x}As$ MDQWs [4, 5]. Recently,

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Freire *et al* [8] have calculated the interface effects in doped nonabrupt GaAs/$Al_xGa_{1-x}As$ single quantum wells. However, they assumed a homogeneous carrier distribution in the structure, allowing only an approximated parabolic representation of their band bendings. Anyway, Freire *et al* [8] obtained that the interface effects on the energy levels are important and sensitive to the level of doping inside the well.

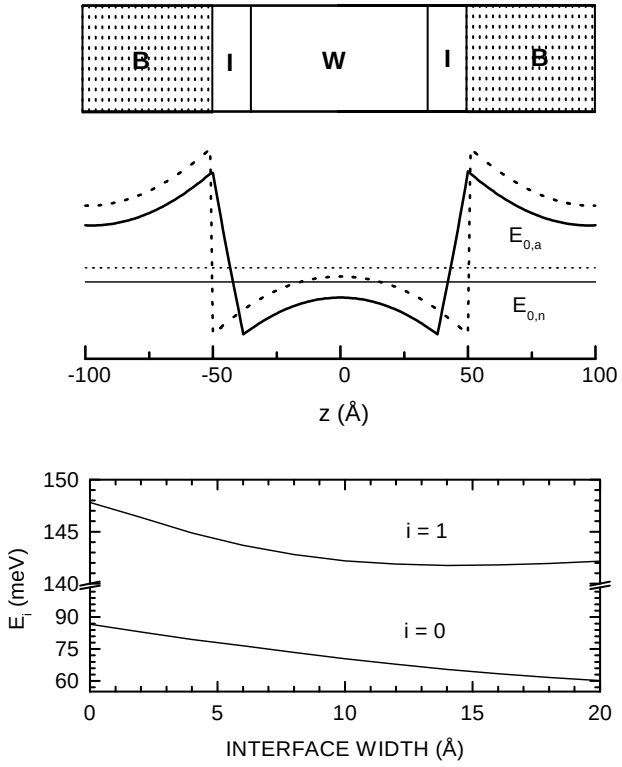

Figure 1. Top: a schematic diagram of the doped GaAs/$Al_{0.3}Ga_{0.7}As$ single quantum well: the regions **B** are the doped $Al_{0.3}Ga_{0.7}As$ barrier regions (shaded regions); the regions **I** are the undoped $Al_xGa_{1-x}As$ interface regions; and the region **W** is the undoped GaAs well region. Middle: the effective potential for a doped abrupt (dotted) and a nonabrupt (solid) GaAs/$Al_{0.3}Ga_{0.7}As$ single quantum well, and their respective ground-state energy levels $E_{0,a}$ and $E_{0,n}$, respectively. Bottom: the interface width dependence of the ground ($i = 0$) and first excited ($i = 1$) electron energy levels of a 100 Å GaAs/$Al_{0.3}Ga_{0.7}As$ single quantum well whose barriers have a doping level of 5×10^{18} cm^{-3}.

In this work, we study how the band-bending effects related to the existence of nonabrupt interfaces change the electron intersubband transitions in modulation-doped GaAs/$Al_xGa_{1-x}As$ single quantum wells. To calculate the electron energy levels, we have self-consistently solved the Poisson and Schrödinger equations for the nonabrupt MDQW. We have also calculated the electron energy levels of an abrupt doped well for the sake of comparison. A schematic representation of our structure is presented at the top of figure 1. It consists of a single nonabrupt GaAs quantum well (with central and interfacial regions **W** and **I**, respectively) sandwiched between two $Al_xGa_{1-x}As$ barriers (only a portion of the barrier regions is shown in the figure, as the shaded regions **B**), whose doping distribution $N_d(z)$ is given by $N_d(z) = N_d$ for $l_w/2 < |z| < l_b + l_w/2$, and $N_d(z) = 0$ otherwise, with z being the GaAs/$Al_xGa_{1-x}As$ MDQW growth direction; N_d is the 3D doping density,

l_w is the total width of the abrupt quantum well, l_b is the width of the doped parts of the Al$_x$Ga$_{1-x}$As barriers, and a is the width of the quantum well interfaces.

Disregarding DX centre effects, the electron effective confinement potential $V_{eff}(z)$ in our MDQW structure consists of the following three contributions [9–11]:

$$V_{eff}(z) = V_H(z) + V_{xc}(z) + V_w(z) \tag{1}$$

where: $V_H(z)$ is the Hartree potential, which is due to the electrostatic interaction of the electrons with themselves and with ionized impurities; $V_{xc}(z)$ is the exchange–correlation potential describing many-body corrections, which is a function of the electron density and can be evaluated within the local-density approximation; and $V_w(z)$ is the nonabrupt quantum well potential, which is parabolic in the interface regions since the difference between the Al$_x$Ga$_{1-x}$As and GaAs band-gap energies in the Γ direction is given by [12]

$$1.155x(z) + 0.37[x(z)]^2$$

and the interface aluminium molar fraction variation is assumed to have a linear dependence on z, as in the previously proposed interfacial description given by Freire *et al* [13, 14].

In the Schrödinger-like equations describing the GaAs/Al$_x$Ga$_{1-x}$As MDQW, the position-dependent kinetic energy operator of BenDaniel and Duke [15] is used to take into account the spatial dependence of the electron effective mass [13, 14], especially in the interfacial regions. During the multistep solution of the Schrödinger equations using the method of Ando and Itoh [16], continuity conditions are imposed on the electron wave function $\Psi(z)$ and on $[m(z)]^{-1}\,\mathrm{d}\Psi(z)/\mathrm{d}z$ at each border of the steps into which the well potential is divided. In the calculations, we have taken the width l_w of the abrupt MDQW as 100 Å, the width l_b of the doped parts of the barriers as 100 Å, and the aluminium molar content in the Al$_x$Ga$_{1-x}$As alloy as $x = 0.3$. The electron band offset is $Q_e = 0.6$, which produces a well depth of $V_x = 227.9$ meV when the barriers are not doped [13, 14].

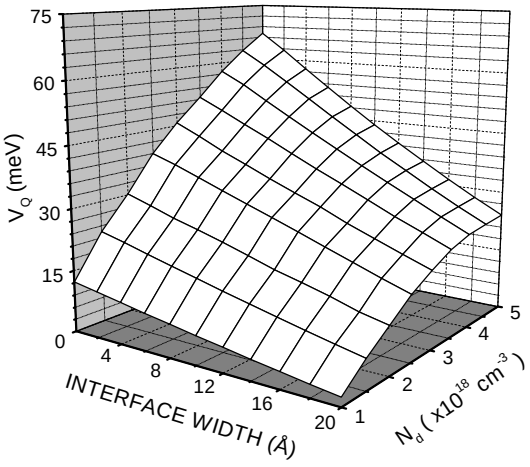

Figure 2. The dependence of the maximum band bending V_Q of the electron self-consistent potential inside a GaAs/Al$_{0.3}$Ga$_{0.7}$As single quantum well 100 Å wide on the interface width and on the barrier doping level.

As a consequence of the existence of nonabrupt interfaces, not only does the depth of the electron effective potential $V_{eff}(z)$ turn out to be smaller, but so also does the band bending inside the well. This is shown in the middle of figure 1, obtained for a barrier doping of 5×10^{18} cm^{-3} and interface widths of 0 Å and 12 Å. In this figure, we can compare the nonabrupt effective potential with the abrupt one, and we observe that the abrupt-interface picture produces an overestimate of the electron energy levels in real samples since they are actually nonabrupt. In fact, the ground-state energy $E_{0,a} = 86.3$ meV for the doped

GaAs/$Al_{0.3}Ga_{0.7}$As abrupt quantum well is higher than $E_{0,n} = 67.8$ meV, the ground-state energy for the doped GaAs/$Al_{0.3}Ga_{0.7}$As nonabrupt quantum well. At the bottom of figure 1, we observe the dependence of the ground ($i = 0$) and first excited ($i = 1$) electron energy levels in a 100 Å GaAs/$Al_{0.3}Ga_{0.7}$As quantum well on its interface width. It is remarkable that an interface width of only 12 Å (which is of the order of the interfacial width in actual samples) can decrease the ground and first excited electron energy levels by as much as 19 meV and 4 meV, respectively, when the level of doping in the barriers is 5×10^{18} cm^{-3}. This result indicates that interfacial effects can be used to explain disagreements of the order of 10 meV between experimental results and theoretical calculations of the electron energy levels in GaAs/Al_xGa_{1-x}As MDQWs.

The reduction of the maximum band bending V_Q of the electron self-consistent potential inside the well changes with the level of doping and with the interface width of the nonabrupt well, as depicted in figure 2. If compared with the band bending of an abrupt well, V_Q can be reduced by as much as 6.4 meV and 27.5 meV by interfaces as thin as 12 Å when the barrier doping levels are 1×10^{18} cm^{-3} and 5×10^{18} cm^{-3}, respectively. This result suggests that calculations based on the abrupt-interface picture can give a good estimate of actual MDQW band bendings only if the doping density in the samples is underestimated, or if the well width is considered to be narrower.

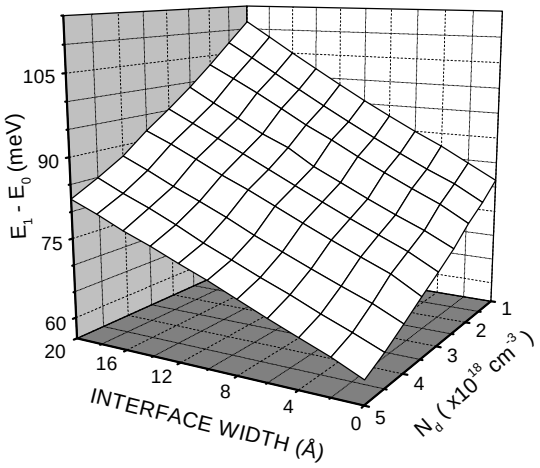

Figure 3. The dependence of the first intersubband transition energy $E_1 - E_0$ of a GaAs/$Al_{0.3}Ga_{0.7}$As single quantum well 100 Å wide on the interface width and on the barrier doping level.

When the barrier doping is increased, the mean well depth becomes smaller and the electron energy levels are higher. However, the rate at which the first electron excited state becomes higher due to the increase of the doping level is smaller than that at which the ground electron state becomes higher. Consequently, the difference $E_1 - E_0$ for the first electron intersubband transition decreases when the doping becomes higher, as shown in figure 3. On the other hand, $E_1 - E_0$ increases when the interface width of the MDQW grows. Compared with the value of $E_1 - E_0$ for the abrupt MDQW, an increase by as much as 17.3 meV and 14.3 meV can be induced by interfaces as thin as 12 Å when the barrier doping levels are 1×10^{18} cm^{-3} and 5×10^{18} cm^{-3}, respectively.

The existence of nonabrupt interfaces in the doped GaAs/$Al_{0.3}Ga_{0.7}$As single quantum well helps also to populate its excited states. This is shown in figure 4 for doping densities

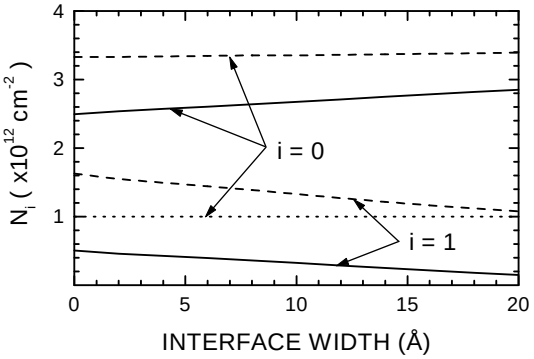

Figure 4. The electron populations in the ground ($i = 0$) and in the first excited ($i = 1$) energy states as functions of the interface width of a GaAs/Al$_{0.3}$Ga$_{0.7}$As single quantum well 100 Å wide whose doping levels in the barriers are 1×10^{18} cm^{-3} (dotted line), 3×10^{18} cm^{-3} (solid lines), and 5×10^{18} cm^{-3} (dashed lines).

of 1×10^{18} cm^{-3} (dotted line), 3×10^{18} cm^{-3} (dashed lines), and 5×10^{18} cm^{-3} (continuous lines). In the case of the smallest level of doping, the population of the ground state remains almost unchanged when the quantum well interface widths increase, since the electron population of the first excited level is very low. When the doping in the barriers is 3×10^{18} cm^{-3}, both the ground and the first excited energy level are populated. But, while the electron population of the ground state becomes higher when the interface width increases, the opposite occurs with the electron population of the first excited state. In the case of the highest level of doping, since the population of the ground state is almost saturated, its population does not change very much when the interface width increases. This is not the case for the electron population of the first excited state, which decreases strongly when the interface is thicker, since for the highest doping level the second excited electron energy levels begin to be populated.

In conclusion, we have demonstrated that intersubband transitions in doped nonabrupt GaAs/Al$_x$Ga$_{1-x}$As single quantum wells are highly dependent on their interface widths. The interface-related band-bending effects can increase the intersubband transition energy by more than 14 meV when the barrier doping levels are as high as 1×10^{18} cm^{-3} and the interface widths are only four monolayers—i.e., the width of the interfaces of actual GaAs/Al$_x$Ga$_{1-x}$As MDQW samples. Although our results need to be compared with experimental results, they lead us to make the suggestion that to achieve a match better than within 5 meV of the measured and calculated energy levels in GaAs/Al$_x$Ga$_{1-x}$As MDQWs, an interface characterization of the samples should always be performed, and must furnish a good estimate of their widths. Finally, the theoretical model to be used for the theoretical description of optical transitions in GaAs/Al$_x$Ga$_{1-x}$As MDQWs should take into account the existence of nonabrupt interfaces in the samples.

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References

[1] Levine B F 1992 *Advanced Research Workshop on Intersubband Transitions in Quantum Wells (NATO ASI Series B: Physics, vol 288)* ed E Rosencher, B Vinter and B F Levine (New York: Plenum) p 43

[2] Educato J L and Leburton J P 1994 *Phys. Rev.* B **49** 2177

[3] Pinczuk A, Störmer H L, Dingle R, Worlock J M, Wiegmann W and Gossard A C 1979 *Solid State Commun.* **32** 1001

In this work, they presented the first experimental observations of the intersubband excitations in GaAs/Al_xGa_{1-x}As MDQWs, explaining them with theoretical calculations based on an abrupt-interface model that produced an agreement not better than or of the order of 5 meV.

[4] Fishman G 1983 *Phys. Rev.* B **27** 7611

[5] Ramsteiner M, Ralston J D, Koidl P, Dischler B, Biebl H, Wagner J and Ennen H 1990 *J. Appl. Phys.* **67** 3900

[6] Johnson M B, Maier U, Meier H P and Salemink H W M 1993 *Appl. Phys. Lett.* **63** 1273

[7] Albrektsen O, Arent D J, Meier H P and Salemink H W M 1990 *Appl. Phys. Lett.* **57** 31

[8] Freire A K, Farias G A, Freire V N and Ferreira E C 1998 *Superlatt. Microstruct.* **23** 1015

[9] Ando T 1982 *J. Phys. Soc. Japan* **51** 3893

[10] Bastard G 1988 *Wave Mechanics Applied to Semiconductor Heterostructures* (New York: Halsted)

[11] Shi J M, Koenraad P M, van de Stadt A F W, Peeters F M, Devreese J T and Wolter J H 1996 *Phys. Rev.* B **54** 7996

[12] Adachi S 1985 *J. Appl. Phys.* **58** R1

[13] Freire V N, Auto M M and Farias G A 1992 *Superlatt. Microstruct.* **1** 17

[14] Freire A K, Ferreira E C, Farias G A and Freire V N 1996 *Superlatt. Microstruct.* **20** 1

[15] BenDaniel D J and Duke C B 1966 *Phys. Rev.* **152** 683

[16] Ando Y and Itoh T 1987 *J. Appl. Phys.* **61** 1497