

Evidence of a two-dimensional to three-dimensional transition in Si δ -doped GaAs structures

C. A. C. Mendonça, F. Plentz, J. B. B. Oliveira, and E. A. Meneses

Instituto de Física, Universidade Estadual de Campinas, 13081-970, Caixa Postal 6165, Campinas, São Paulo, Brazil

L. M. R. Scolfaro, D. Beliaev, S. M. Shibli, and J. R. Leite

Instituto de Física, Universidade de São Paulo, 01498-970, Caixa Postal 20516, São Paulo, São Paulo, Brazil

(Received 26 April 1993)

We report on the change of character, from an “isolated” well to a superlattice, of multiple δ -doped structures as a function of the doping period d_s . This effect is evidenced by the drastic change in the photoluminescence excitation spectra and the deviation on the total electron density extracted from Shubnikov-de Haas oscillation measurements as d_s decreases. Self-consistent-calculation results performed for these systems are used for comparison.

Multiple δ -doped GaAs structures have been widely investigated lately.¹⁻⁸ The variation of the doping period, d_s , has been shown to strongly affect the properties of such systems. Results from self-consistent calculations, based on the design parameters, have shown that the characteristic energy level scheme of an isolated δ potential is replaced by a set of minibands of finite width, reflecting a superlatticelike behavior, when d_s decreases.^{3,7}

From the experimental point of view, optical techniques, such as photoluminescence (PL), have proved to be extremely useful in the study of the properties of such structures. Effects associated to miniband formation and confinement of photogenerated holes, as d_s decreases, have been reported.⁵⁻⁸

In this work we report on the experimental observation of a change in character of these systems, from quasibidimensional (isolated δ well) to tridimensional (δ -superlattice). The combination of photoluminescence excitation spectroscopy (PLE) with the transport (Shubnikov-de Haas oscillations) measurements allows us to avoid misleading interpretations of the data. To reinforce our point of view we also show results of a self-consistent calculation based on the transport results.

The multiple δ -doped samples were grown by molecular beam epitaxy (MBE), on (100)GaAs semi-insulating substrates. The temperature was 540 °C to minimize Si diffusion and segregation.¹ The growth rate determined from the reflection high-energy electron-diffraction (RHEED) oscillations was 1.1 μ /h. The “stop-and-go” procedure, which was used to introduce a dopant plan, was repeated to provide the periodic structures, with a nominal Si atoms sheet concentration of 3×10^{12} cm⁻². The width of the intrinsic GaAs layer separating adjacent dopant plans was varied from 40 to 1000 Å, and the resulting structures consist of 50–100 periods.

PLE measurements were performed with the samples immersed in superfluid He (2 K). The excitation source in the PLE experiments was a Kr⁺ pumped LD 700 tunable ring dye laser. The emission spectra were analyzed with a 0.75-m double monochromator and detected by a liquid nitrogen cooled S1 photomultiplier and an electrome-

ter. The magnetotransport measurements were also performed at 2 K, in a Nb₃Sn magnet, in which magnetic fields varied from 0 to 14 T. The field was applied in the direction perpendicular to the sample surface.

Figure 1 shows the PLE spectra for the samples with $d_s \leq 220$ Å. Two aspects are to be remarked when d_s decreases. The first is the strong blueshift shown by the profile in the spectra. The other aspect is the drastic change in their line shape with the variation of the doping period. While for the structure with $d_s = 220$ Å the absorption profile is steep, it becomes smoother for the samples with shorter period structures. These phenomena can be associated to those observed in PL experiments in the same samples.^{5,6} We will consider the energy at half maximum of profile as a reference and will define it as the absorption onset.

The results from Shubnikov-de Haas measurements for the samples with $d_s = 100, 160,$ and 400 Å, represented by their Fourier power spectra, are shown in Figs. 2(a)–

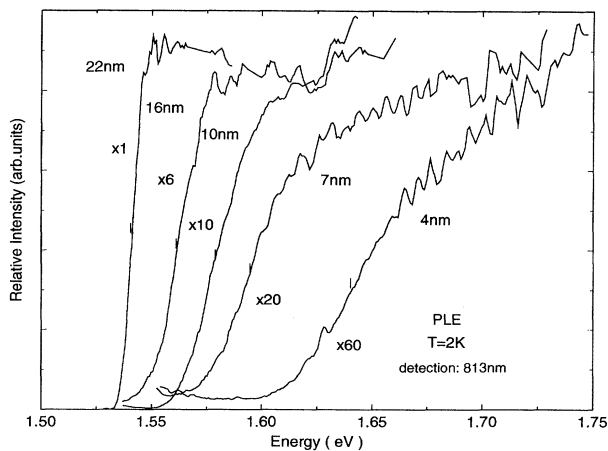


FIG. 1. PLE spectra for the multiple δ -doped structures with $d_s \leq 220$ Å. The absorption onset energy is marked by arrows in the half maximum of the profile.

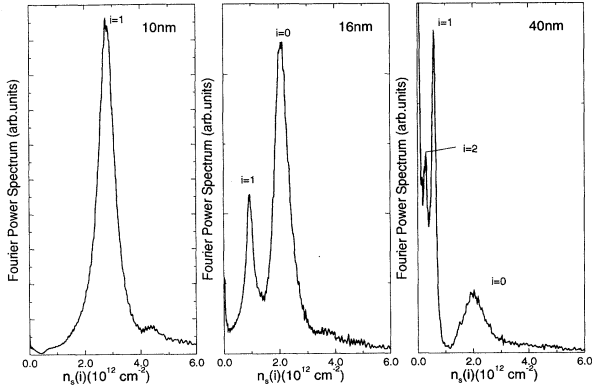


FIG. 2. Fourier power spectrum as a function of n_s , for the samples with $d_s = 100, 160,$ and 400 \AA . The subband index associated with the structure is shown in the figure.

2(c). Each structure in the spectra is associated to the occupancy of one electron subband. It can be noticed that, the longer the period of the superlattice is, the more structures can be distinguished in the spectra. While for $d_s = 100 \text{ \AA}$ only one subband is occupied, for $d_s = 160$ and 400 \AA we observe the occupation of two and three subbands, respectively.

In Fig. 3 we show the dependence on d_s of the total two-dimensional electron gas (2DEG) density and the partial subband occupancies obtained from magnetotransport experiments. It can be observed that, for $d_s \geq 150 \text{ \AA}$, the sum of the partial subband occupancies results in a 2DEG density around $3 \times 10^{12} \text{ cm}^{-2}$, which is the nominal value for the dopant sheet density. For d_s lower than 150 \AA , we found higher values for the electron gas density. This results indicate that a 2D to 3D transition occurs when the doping period is decreased in multiple δ -doped structures.

Self-consistent one-electron-state calculations were performed, in which the input parameters were the ex-

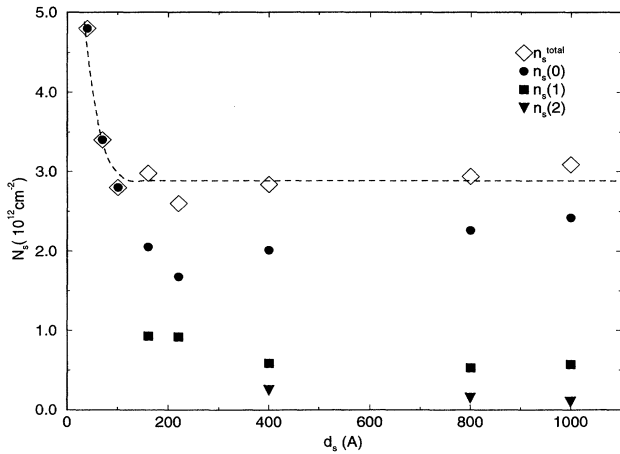


FIG. 3. Dependence on d_s , of the total 2DEG, given by $n_s = \sum_{i=0}^N n_s(i)$ and of the partial subband occupancies $n_s(i)$, obtained from the magnetotransport measurements.

perimental 2DEG density and the design period of each structure. The calculations are based on a simultaneous solution of the Schrödinger equation in the effective mass approximation, and the Poisson equation. The periodicity of the screened potential along the direction perpendicular to the plans of ionized donors leads to electronic wave functions which are products of plane waves by one-dimensional Bloch states.³ The one-dimensional Schrödinger equation is solved by adopting the Wigner-Seitz-Slater version of the cellular method with space filling one-dimensional cells and the exact point-match approach.⁹ Exchange-correlation effects within the local density approximation were taken into account, using the parametrization of Hedin and Lundqvist.¹⁰ The dopant atoms were assumed to be ionized and uniformly distributed in 10 \AA . The results for the most important characteristics of the multiple δ -doped systems are in Table I. Namely, they are the potential depth V , the Fermi energy E_F , the energy of the bottom of the subbands E_i , and their energy dispersion $\Delta E_i = |E_i(k=0) - E_i(k=\pi/d_s)|$, the energy at the top of the first heavy-hole subband H_0 , and its width ΔH_0 . It can be noticed that the miniband that originated from the fundamental energy level for electrons, E_0 , starts to present significant width for $d_s \approx 160 \text{ \AA}$. For the holes this limit is lower, with the width of the first heavy-hole subband greater than 10 meV being observed only for $d_s < 70 \text{ \AA}$.

From the results of the self-consistent calculations it is possible to estimate the theoretical absorption onset using

$$h\nu^{\text{onset}} = E_G^{\text{GaAs}} - V + E_F + H_F, \quad (1)$$

where E_G^{GaAs} is the fundamental GaAs band-gap energy (1.5192 eV) and H_F is the quasi-Fermi-level for photo-generated holes, taken to be equal to the first heavy-hole energy, H_0 . The values of V , E_F , and H_F are those extracted from the calculations. A comparison between the experimental and theoretical values for $h\nu^{\text{onset}}$ is shown

TABLE I. Characteristics of the multiple δ -doped structures, extracted from the self-consistent calculations. V , E_F , E_i , ΔE_i , H_0 , and ΔH_0 are given in meV. In the calculations, the densities of dopant ions and of the 2DEG are those obtained from the Shubnikov-de Haas measurements, i.e., $n_s = \sum_{i=0}^N n_s(i)$.

d_s (Å)	1000	800	400	220	160	100	70	40
V	122.3	117.8	109.2	88.3	82.4	61.8	57.5	49
E_F	121.7	117.7	114.6	107.9	118.2	116.9	149.1	192.5
E_0	48.5	47	46.5	43	43.6	33.6	29.4	23.5
ΔE_0	0	0	0	2	9	43	101	332.5
E_1	97.5	94.6	92	92	87.9	102.6	-	-
ΔE_1	0	0	1.3	21.4	51.4	154	-	-
E_2	112.8	109.5	105	106.9	136	254	-	-
ΔE_2	0	0.1	8.3	51.4	105	274	-	-
E_3	120	116.1	-	-	-	-	-	-
ΔE_3	0.5	1.9	-	-	-	-	-	-
H_0	0.9	1.5	5.3	11	13.8	19.1	22.9	24
ΔH_0	0	0	0	0	0	1.6	7.7	41.6

in Table II.

The blueshift in the PLE spectra is attributed to the Fermi level displacement into the conduction band, due to the enhancement of the effective doping level, and the increase in the hole confinement energies with the decrease of the structure period. In this sense, this effect can be directly related to the increase of the absorption onset, $h\nu^{\text{onset}}$, for decreasing doping period. The quantitative discrepancy between the theoretical and the experimental values for $h\nu^{\text{onset}}$, observed in Table II, are due to the value of E_G^{GaAs} considered in Eq. (1). By taking the fundamental GaAs band-gap energy, many-body effects, such as the shrinkage of the band gap in heavily doped materials,¹¹ are neglected.

The fundamental aspect of our work is related to the anomalous behavior of the measured 2DEG total density versus d_s , for short doping periods (see Fig. 3). The determination of the 2DEG density is based on a strictly 2D treatment of the Shubnikov–de Haas oscillations. The deviation of the measured density from the nominal dopant sheet concentration for d_s lower than 150 Å, indicates that the model used fails to describe multiple δ -doped systems with short periods. We attribute this effect to a transition from a 2D to a 3D regime in multiple δ -doped structures with short spacing layer between consecutive dopant sheets, resembling their superlattice character. These results are corroborated by those obtained from PLE measurements. The modification in the absorption line shape is due to the miniband formation when the adjacent wells are coupled. In this case, the density of states strongly deviates from steplike (2D) and approaches that of a 3D system (superlattice). In this sense, the steep onset of the absorption observed in the PLE spectrum for $d_s = 220$ Å is closer to what is expected for a 2D system, as a quantum well. On the other hand, in the spectrum

TABLE II. Comparison between theoretical values of the absorption onset estimated from Eq. (1) and those obtained from PLE spectra.

d_s (Å)		220	160	100	70	40
$h\nu^{\text{onset}}$ (eV)	expt.	1.541	1.563	1.585	1.601	1.662
	theor.	1.550	1.568	1.593	1.634	1.687

for $d_s = 40$ Å the absorption profile approaches the one expected for a 3D system. This aspect is reinforced by the self-consistent calculation results for the miniband widths. The extreme situation is reached when both ΔE_i and ΔH_0 assume considerable values (>10 meV). This is the case of the structures with $d_s = 40$ and 70 Å, in which the 3D character is clearly identified.

In summary, a 2D to 3D transition is shown to take place when the doping period, in multiple δ -doped structures, is decreased. The anomalous dependence of the 2DEG total density on d_s and remarkable change in the absorption line shape, sustain this assumption, which is also reinforced by results from self-consistent calculations. Additional evidence of the 2D-3D transition (miniband formation) could be given by SdH measurements in tilted magnetic field.^{12,13} The miniband formation can be extracted directly from the examination of the PLE measurements, which reflect the change of the density of states when we undergo to the observed 2D-3D transition.

The authors would like to acknowledge CAPES, CNPq, and FAPESP (Brazilian funding agencies) for financial support.

¹ E.F. Schubert, Surf. Sci. **228**, 240 (1990), and references therein.

² A.C. Maciel, M. Tatham, J.F. Ryan, J.M. Worlock, R.E. Nahory, J.P. Harbison, and L.T. Florez, Surf. Sci. **228**, 251 (1990).

³ M.H. Degani, J. Appl. Phys. **70**, 4362 (1991).

⁴ J.C. Egues, J.C. Barbosa, A.C. Notari, P. Basmaji, L. Iorriatti, E. Ranz, and J.C. Portal, J. Appl. Phys. **70**, 3678 (1991).

⁵ S.M. Shibli, L.M.R. Scolfaro, J.R. Leite, C.A.C. Mendonça, F. Plentz, and E.A. Meneses, Appl. Phys. Lett. **60**, 2895 (1992).

⁶ C.A.C. Mendonça, L.M.R. Scolfaro, A.B. Henriques, J.B.B. Oliveira, F. Plentz, S.M. Shibli, E.A. Meneses, and J.R.

Leite (unpublished).

⁷ M. Ke, J.S. Rimmer, B. Hamilton, J.H. Evans, M. Missous, K. Singer, and P. Zalm, Phys. Rev. B **45**, 14 114 (1992).

⁸ M. Ke, J.S. Rimmer, B. Hamilton, M. Missous, B. Kumshepour, J.H. Evans, K.E. Singer, and P. Zalm, Surf. Sci. **267**, 65 (1992).

⁹ J.R. Leite, B.I.O. Bennett, and F. Herman. Phys. Rev. B **12**, 1466 (1975).

¹⁰ L. Hedin and B.I. Lundqvist, J. Phys. C **4**, 2064 (1971).

¹¹ G.E.W. Bauer, Surf. Sci. **229**, 374 (1990).

¹² L.L. Chang, E.E. Mendez, N.J. Kawai, and L. Esaki, Surf. Sci. **113**, 306 (1982).

¹³ H.L. Störmer, J.P. Eisenstein, A.C. Gossard, W. Wiegmann, and K. Baldwin, Phys. Rev. Lett. **56**, 85 (1986).