GaSb-InAs-GaSb heterostructures studied under hydrostatic pressure

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We report transport measurements on GaSb-InAs-GaSb heterostructures under hydrostatic pressure (up to 1.2 GPa) and high magnetic field (up to 18 T) at low temperature. The pressure-induced decrease of the carrier concentrations is analyzed in terms of two distinct causes: an intrinsic charge transfer between the GaSb valence band and InAs conduction band, and an electron transfer to interface donor states. Using a simple self-consistent variational approach to model the structure and the experimental values of the concentration rates of decrease, we are able to estimate (1) the effective rate at which the band discontinuity Δ at the interface decreases as we apply pressure $(d\Delta/dP = 67$ meV/GPa) and (2) the density of interface states $(n_T \approx 4 \times 10^{12}$ cm^{-2} eV$^{-1})$. Nonparabolicity of the InAs conduction band has been taken into account in the calculations.

INTRODUCTION

We have recently given evidence of a semimetal-semiconductor transition induced by hydrostatic pressure on a GaSb-InAs-GaSb double heterostructure with an InAs thickness of $L = 150$ Å.[1] An intrinsic charge transfer occurring between the valence band of GaSb and the conduction band of InAs (see Fig. 1) is responsible for the semimetallic character of this system, but the contribution of another source of electrons, presumably interface donor states,[2,3] has to be invoked to explain the fact that the electron concentration is larger than that of the holes.[3] As we apply pressure, the InAs conduction band goes upward in energy, causing a decrease of the band discontinuity Δ between the GaSb valence band and InAs conduction band at the interface. In the semimetallic regime, this brings about a reduction of the intrinsic charge transfer leading to a complete elimination of the hole gas, i.e., to a semimetal-semiconductor transition.

The study will here be extended to samples having $L = 70$ and 100 Å, where the conduction is due to electrons only (i.e., these samples are already in the semiconductor regime at ambient pressure). Using a simple self-consistent variational approach to model the structure, we will obtain the value of the effective decrease rate $d\Delta/dP$ of the potential discontinuity and an estimation of the density of interface states necessary to explain the observed decrease in the electron concentration with pressure. Calculations have been done with and without taking the nonparabolicity of the InAs conduction band into account, in order to gauge the influence of nonparabolicity on the quantitative interpretation of the results.

EXPERIMENTAL RESULTS

Using the liquid-pressure-cell technique, we have performed Hall and Shubnikov–de Haas measurements under hydrostatic pressure up to 1.2 GPa at 4.2 K. Typical curves are reported in Fig. 2 for the sample with $L = 70$ Å. Hall plateaus and zero resistivities are well observed and shift with pressure due to the decrease in the electron concentration. For this sample, as well as the $L = 100$-Å one (not shown), there is no evidence of extra features on $\rho_{xx}(B)$ and $\rho_{xy}(B)$ nor of a positive curvature of $\rho_{xy}(B)$ at low field, which are the signatures of conduction by both electron and hole gases.[1,3] We thereby conclude that these two samples are in their semiconducting state and we attribute the decrease of $N_e(P)$ to a transfer of electrons into unoccupied interface donor states. As can be noted on Fig. 3(a), the decrease rates of $N_e(P)$ are equal for these two samples $(dN_e/dP = -2.4 \times 10^{11}$ cm^{-2} GPa$^{-1})$ as well as for the sample with $L = 150$ Å when it has reached its semiconducting regime $(P > 0.85$ GPa). For the semimetallic case $(L = 150$ Å, $P < 0.85$ GPa), N_e decreases faster $(dN_e/dP = -3.6 \times 10^{11}$ cm^{-2} GPa$^{-1})$, due to the contribution of the intrinsic transfer. A mobility rise with pressure [Fig. 3(b)] is observed only for the $L = 150$-Å sample for $P < 0.85$ GPa and can be associated with the decrease of the hole concentration.

THEORY

We will basically use the variational self-consistent approach developed by Bastard *et al.*[4] The main difference with these authors will be in our choice of the electron's variational wave function. We first describe our approach considering the InAs conduction band to be parabolic; the way nonparabolicity is introduced will be given afterward.

Let us define the potential energy $V(z)$ as

$$V(z) = \begin{cases} -e\phi(z) + \Delta, & |z| > L/2 \\ -e\phi(z), & |z| < L/2, \end{cases} \tag{1}$$

(a)

E

E_B

E_A

GaSb   InAs   GaSb

μ E_e

L
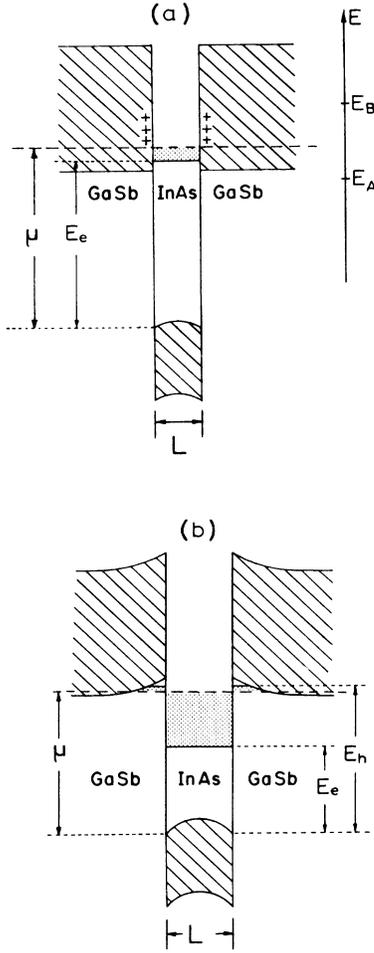
(b)

μ

GaSb   InAs   GaSb E_e

E_h

L

FIG. 1. Energy-band diagram of GaSb-InAs-GaSb double heterostructure (a) in the semiconductor regime, where all the electrons are provided by interface donor states, and (b) in the semimetallic regime, where an intrinsic charge transfer adds up to interface states as a source of electrons, and brings about the simultaneous presence of two-dimensional electron and holes gases in unequal concentrations. Hatched regions represent the gaps (not to scale). The interface donor states are assumed to be uniformly distributed in the energy interval $[E_A, E_B]$.

where $\phi(z)$ is the electrostatic potential, which enters the Poisson equation:

$$d^2\phi/dz^2 = \begin{cases} eN_e \mid \psi_e(z) \mid^2/\epsilon_e, & \mid z \mid < L/2 \\ -eN_h \mid \psi_h(z) \mid^2/2\epsilon_h, & \mid z \mid > L/2 , \end{cases} \quad (2)$$

where ϵ_e and ϵ_h are the permittivities of InAs and GaSb,

$2k\Omega/\square$ L=70 Å
4.2K   (a)

ρ_{xx}

1.05 GPa

0   0.77 GPa

0   0.49 GPa

0   0.09 GPa

0   5   10   15   20

B (T)

30   L=70 Å   (b)
            4.2 K   i=1

25

20   1.05 GPa   0.09 GPa

ρ_{xy} (kΩ)   15
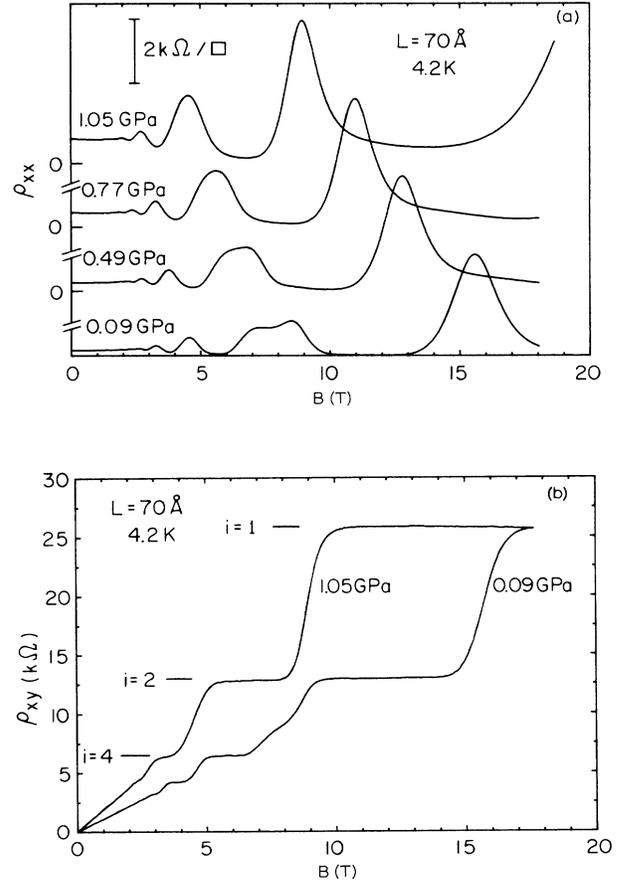
i=2

10

5   i=4

0
0   5   10   15   20

B (T)

FIG. 2. Typical recordings of (a) the resistivity and (b) the Hall resistivity at different pressures for the sample having $L = 70$ Å.

respectively, and N_e is the electron concentration. We suppose the structure to be perfectly symmetrical respective to the center of the InAs layer; therefore the hole concentration is the same in each hole well, and N_h represents the total concentration in these two wells.

The Schrödinger equation is written

$$[p^2/2m_e^* + V(z)]\psi_e(z) = E_e\psi_e(z), \quad \mid z \mid < L/2$$

$$[p^2/2m_h^* + V(z)]\psi_h(z) = E_h\psi_h(z), \quad \mid z \mid > L/2 , \quad (3)$$

where $\psi_e(z)$ and $\psi_h(z)$ are the envelope functions for the electrons and holes, respectively. m_h^* and m_e^* are the effective masses for the heavy holes in GaSb and for the electrons in InAs.

The variational wave functions used are

$$\psi_e(z) = \begin{cases} (2/L)^{1/2}\cos(\pi z/L), & \mid z \mid < L/2 \\ 0, & \mid z \mid > L/2 , \end{cases} \quad (4)$$

$$\psi_h(z) = \begin{cases} (1/2\alpha^3)^{1/2}(\mid z \mid -L/2)\exp[-(\mid z \mid -L/2)/2\alpha], & \mid z \mid > L/2 \\ 0, & \mid z \mid < L/2 . \end{cases} \quad (5)$$
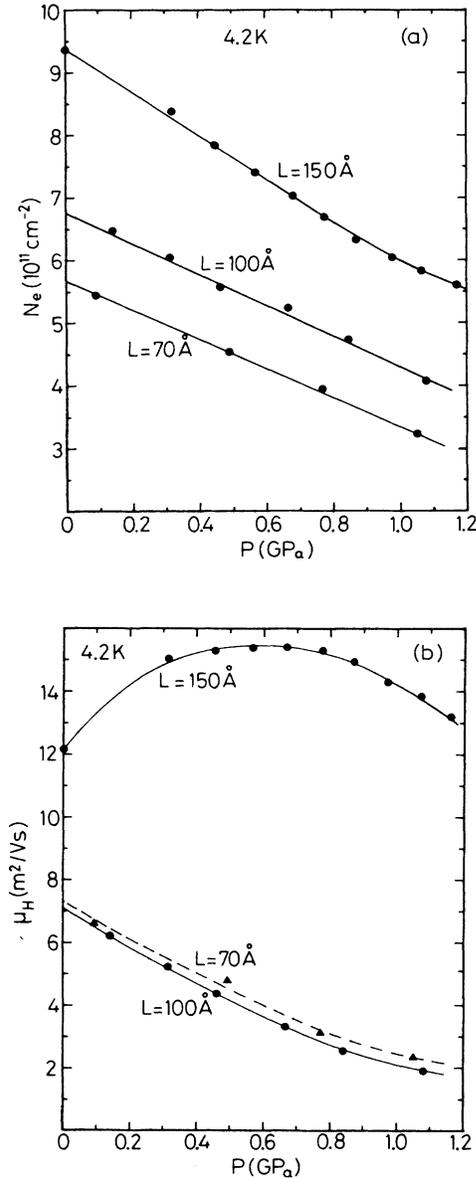
FIG. 3. (a) Electron concentration as deduced from the periodicity of Shubnikov–de Haas oscillations and (b) Hall mobility at several pressures for three different thicknesses of the InAs layer. Curves are just guides for the eye.

$\psi_e(z)$ is the wave function of the fundamental energy level of an infinite square well. By making this choice, we neglect the effect of the bowing of the bottom of the well on $\psi_e(z)$. This leads to a small error compared to the results of Ref. 2 if the well width is small (say < 200 Å).

$\psi_h(z)$ is the Fang-Howard function[5] and α is the variational parameter, which takes the value

$$\alpha = \left[\frac{16\hbar^2\epsilon_h}{33m_h^*e^2N_h}\right]^{1/3} . \tag{6}$$

The energy levels are then given by

$$E_e = \hbar^2\pi^2/2m_e^* L^2 + e^2 N_e L^2(1/12+5/8\pi^2)/\epsilon_e , \tag{7}$$

$$E_h = \Delta - \hbar^2/8m_h^*\alpha^2 - 33N_h e^2\alpha/32\epsilon_h . \tag{8}$$

The constancy of the chemical potential μ imposes that (at $T = 0$ K)

$$\mu = E_e + \pi\hbar^2 N_e /m_e^* \tag{9a}$$

and

$$\mu = E_h - \pi\hbar^2 N_h /2m_h^* , \tag{9b}$$

where we have taken the density of states of each carrier into account. In general we will have $N_e = N_h + \Delta N_t$, where ΔN_t is the contribution of the interface states, which reduces to zero in the ideal case where the electrons are provided exclusively by an intrinsic charge transfer.

This completes the description of our approach in the parabolic approximation. The nonparabolicity of the InAs conduction band can be introduced, in a simplified way, by using the energy-dependent effective mass:

$$m_e^*(E_b) = m_0^*(1+2K_{np}E_b/E_g) \tag{10}$$

with[6]

$$K_{np} = \left[1 - \frac{m_0^*}{m}\right]^2 \frac{3E_g^2+4\Delta_{s-o}E_g+2\Delta_{s-o}^2}{(E_g+\Delta_{s-o})(3E_g+2\Delta_{s-o})} = 0.86 , \tag{11}$$

where m is the free electron mass and m_0^* the conduction-band-edge mass. We have used $E_g = 0.42$ eV, $\Delta_{s-o} = 0.43$ eV, $m_0^* = 0.23$ m, $\epsilon_e = 12.5\epsilon_0$, and $\epsilon_h = 14.8\epsilon_0$. For the mass of the heavy holes, we have taken $m_h^* = 0.33$. E_b is the energy relative to the conduction-band edge and is a function of the position $[E_b(z) = E - E_c(z)]$ because of the bowing of the bottom of the well. If this bowing is small we can write

$$m_e^*(E,z) \simeq m_e^*(E) = m_0^*(1+2K_{np}E/E_g) . \tag{12}$$

This approximation is well justified in our case, and simplifies considerably the calculations.

The only modifications to the parabolic model will therefore consist of writing

$$N_e = \frac{m_0^*}{\pi\hbar^2}\left[\mu\left(1+K_{np}\frac{\mu}{E_g}\right) - E_e\left(1+K_{np}\frac{E_e}{E_g}\right)\right] , \tag{13a}$$

$$N_h = \frac{2m_h^*}{\pi\hbar^2}(E_h - \mu) \tag{13b}$$

instead of Eq. (9), and

$$E_e = \frac{\hbar^2\pi^2}{2m_e^*(E_e)L^2} + \frac{e^2 N_e L^2}{\epsilon_e}\left[\frac{1}{12}+\frac{5}{8\pi^2}\right] \tag{14}$$

instead of Eq. (7).

Despite its simplicity, we will see that this approach is able to give a quantitative support to our interpretation. In practice, the symmetry of the band diagram is most probably broken due to the lifting of the degeneracy of the two holes levels and to the nonequivalent quality of the two interfaces. Although it can bring strong altera-

tions in the details of the magnetoresistance oscillations at high magnetic field for example,[7] this asymmetry should not affect the essence of the conclusions drawn in this paper.

INFLUENCE OF PRESSURE

In the III-V compounds, pressure induces an increase of the gap at the Γ point at a rate which is well known for the most common of these compounds.[8] This, however, involves only the relative position of the conduction- and valence-band edges. In the case of our heterostructures, it would be necessary to know the absolute variation of the valence-band edge in GaSb and of the conduction-band edge in InAs in order to estimate $d\Delta/dP$. These data are not available, but a rough estimation can be made by supposing that the two valence bands remain fixed relatively to each other. In this situation, Δ is expected to vary as the InAs gap: $d\Delta/dP = dE_g$ (InAs)$/dP = -100$ meV/GPa.[8] However, recent optical measurements made on InAs-GaSb superlattices give $d\Delta/dP = -58$ meV/GPa (Ref. 9) and show that both conduction- and valence-band discontinuities are affected by pressure.

Our transport measurements provide an alternate way to estimate $d\Delta/dP$ through the use of the model described above. The only additional quantity needed to make such estimation is the rate of variation of the band-edge mass with pressure in InAs, which has been taken as[10]

$$m_0^*(P) = m_0^*(0) + 6.67 \times 10^{-3} P , \qquad (15)$$

with P in GPa.

DETERMINATION OF $d\Delta/dP$ AND n_T

We will examine separately the two cases where the structure is in a semiconductor state (GaSb valence-band edge below μ) or a semimetallic state (GaSb valence-band edge above μ).

Semiconductor case

Let n_T be the density of interface states per unit area and unit energy for each interface. We suppose this density to be constant in an energy interval $[E_A, E_B]$ (see Fig. 1), and zero elsewhere. Then

$$N_e = \Delta N_t = 2n_T[E_B - \mu - E_c(\text{InAs})] \qquad (16)$$

and the rate of variation of $N_e(P)$ can be written as

$$\frac{dN_e}{dP} = 2n_T \left[\frac{d\Delta}{dP} - \frac{d\mu}{dP} \right] . \qquad (17)$$

Using the value of $d\Delta/dP$ as a parameter, and the experimental value of dN_e/dP, it is possible to obtain $d\mu/dP$ through Eqs. (9a) or (13a), and then the value of n_T using Eq. (17). Results are shown in Fig. 4 for the non-parabolic model with $dN_e/dP = -2.4 \times 10^{11}$ cm^{-2} GPa^{-1}. The order of magnitude obtained for n_T (10^{12} to 10^{13} cm^{-2} eV^{-1}) is quite plausible.[11] These calculations, based on a linear decrease of $N_e(P)$, show that
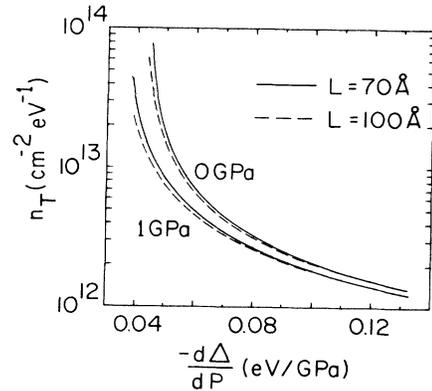

FIG. 4. Concentration of interface donor states needed to obtain $dN_e/dP = -2.4 \times 10^{11}$ cm^{-2} GPa^{-1} as a function of $d\Delta/dP$. Calculations have been made using the nonparabolic approach described in the text.

n_T is not very sensitive to the pressure or the well width, even though the values used for these parameters in Fig. 4 correspond to very different electron concentrations or Fermi energies. This confirms that a linear variation $N_e(P)$ is consistent with the hypothesis of a uniform density of interface states in the energy range we are concerned with here.

In the case of the parabolic model, the value of $d\mu/dP$ needed to obtain the observed dN_e/dP through Eq. (9a) is much larger than in the nonparabolic model because of the smaller density of states of the two-dimensional electron gas. In that situation, a larger $d\Delta/dP$ must be used in order to get a positive value for n_T from Eq. (17). Calculations show that $d\Delta/dP$ must actually be larger than 150 meV/GPa, a value that seems quite unrealistic in this context. We therefore omitted a graphical representation of these theoretical results.

Semimetallic case

Let us first suppose that the interface states possibly present under the GaSb valence-band edge have a negligible influence on the transfer rate. In other words, we suppose that ΔN_t is independent of pressure, and therefore that dN_e/dP depends only on $d\Delta/dP$ as long as the structure is in its semimetallic state. We will see below that this is not a bad approximation. Equations (7), (8), and (9) in the parabolic model, or Eqs. (13), (14), and (8) in the nonparabolic model can be easily solved to obtain N_e as a function of pressure. Results are shown in Fig. 5 for different values of $d\Delta/dP$. We can see that $N_e(P)$ varies almost linearly for any $d\Delta/dP$ and that the inclusion of nonparabolicity strongly affects the decrease rate.

Listed in Table I are the values of $d\Delta/dP$ necessary to obtain $dN_e/dP = -3.6 \times 10^{11}$ cm^{-2} GPa^{-1} (i.e., the experimental value obtained with the sample having $L = 150$ Å) for different Δ and ΔN_t. In the parabolic model, the value of Δ needed to obtain the observed concentrations N_e and N_h at ambient pressure is quite large
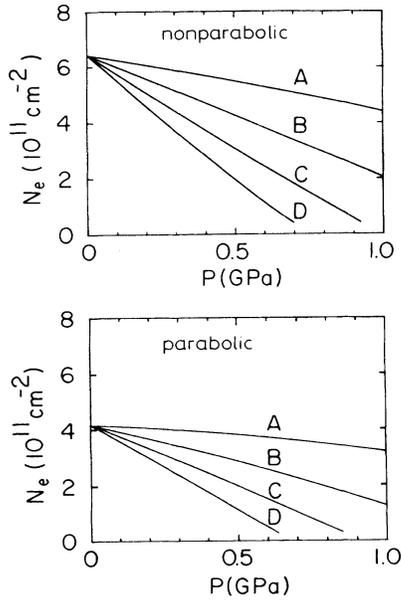
FIG. 5. N_e as a function of pressure, calculated using the self-consistent variational approach for different values of $d\Delta/dP$, assuming $\Delta N_t = 0$. Curve A, $d\Delta/dP = -40$ meV/GPa; curve B, $d\Delta/dP = -70$ meV/GPa; curve C, $d\Delta/dP = -100$ meV/GPa; curve D, $d\Delta/dP = -130$ meV/GPa.

(213 meV) compared to the commonly used value (150 meV), while the value of $d\Delta/dP$ ($= -110$ meV/GPa) is not unrealistic. In the nonparabolic model, a good agreement is obtained with plausible values for both Δ ($= 163$ meV) and $d\Delta/dP$ ($= -67$ meV/GPa). Note that the latter value is in nice agreement with the result of optical measurements,[9] but is significantly lower than $dE_g(\text{InAs})/dP$. Some detailed calculations including strain effects and couplings between bands would be needed to determine the cause of this difference.

Positions of the different energy levels E_e, E_h, and μ as a function of the well width are plotted in Fig. 6. In the case where $\Delta N_t = 0$, these curves indicate that the semimetal-semiconductor transition occurs around $L = 85$ and 105 Å, respectively, in the nonparabolic and the parabolic approaches. When conditions C of Table I are used for the calculations, ie., when the contribution of interface states is included, we find 105 and 115 Å, respectively. This is interesting since it shows that for the two narrower wells ($L = 70$ and 100 Å), we obtain that no holes should be present, as it is observed experimentally in our samples. However, more recent measurements have shown that holes can be present for L as low as 60 Å.[12] As suggested by preliminary estimations,[7] strain effects are possibly a cause of such a reduction in the critical value of L corresponding to the semimetal-semiconductor transition compared to our results. The fact that we do not observe the presence of holes for $L = 70$ and 100 Å could presumably be attributed to a larger density of interface states in our samples, compared to the higher quality samples used in Ref. 12.

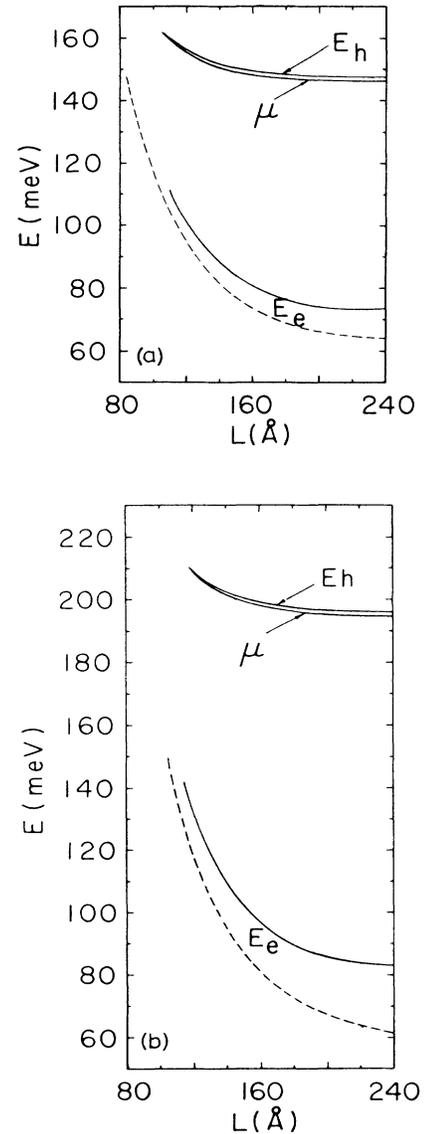In practice, interface states might well be located

FIG. 6. Solid lines give the position of the energy levels E_e, E_h, and μ as a function of InAs thickness L using conditions (C) of Table I for the values of Δ and ΔN_t. (a) Parabolic model and (b) nonparabolic model. Dashed lines give, for comparison, the position of the electron quantized level E_e when conditions (A) of Table I are used for the calculations.

below the valence-band edge of GaSb. In that case, we have to consider those states in addition to the intrinsic charge transfer in our calculations of the carrier concentration as a function of pressure. This can be done by writing

$$N_e = N_h + \Delta N_{t0} + 2[E_v(\text{GaSb}) - \mu]n_T , \qquad (18)$$

where ΔN_{t0} is the contribution of the interface states located above $E_v(\text{GaSb})$ only, and we have assumed that

TABLE I. Calculated values of $d\Delta/dP$ needed to obtain $dN_e/dP = -3.6\times10^{11}$ cm^{-2}GPa^{-1} for $L = 150$ Å in the parabolic and nonparabolic model. N_{e0} and N_{h0} are the carriers obtained at $P = 0$ GPa in the following conditions: (A) $\Delta N_t = 0$ is assumed and the commonly used value of Δ is taken. (B) ΔN_t is adjusted in order to obtain the observed hole concentration $N_{h0} = 2.35\times10^{11}$ cm^{-2}. (C) ΔN_t and Δ are fitted to obtain an agreement with observed values of both N_{e0} and N_{h0}.

Condition	Δ (meV)	ΔN_t (10^{11} cm^{-2})	N_{e0} (10^{11} cm^{-2})	N_{h0} (10^{11} cm^{-2})	$d\Delta/dP$ (meV/GPa)
		Parabolic model			
(A)	150	0	4.22	4.22	−92
(B)	150	2.4	4.75	2.35	−96
(C)	213	7.0	9.35	2.35	−110
		Nonparabolic model			
(A)	150	0	6.41	6.41	−63
(B)	150	5.35	7.7	2.35	−67
(C)	163	7.0	9.35	2.35	−67

the density n_T is uniform. In the wider well, the value of dN_e/dP now depends on both $d\Delta/dP$ and n_T, as in the narrower wells. Using the values of dN_e/dP corresponding to the semiconductor and semimetallic cases, we can evaluate $d\Delta/dP$ and n_T from Eqs. (17) and (18). ΔN_{t0} is adjusted to obtain a quantitative agreement with the experiment for N_e and N_h at ambient pressure. We found that the set of values $d\Delta/dP = -67$ meV/GPa, $\Delta N_{t0} = 6\times10^{11}$ cm^{-2}, and $n_T = 4\times10^{12}$ cm^{-2}eV^{-1} gives a consistent description in good agreement with all our results. These values are close to the ones found above, and this shows that the intrinsic charge transfer dominates strongly over the contribution from interface states. Considering this density of interface states, an evaluation of E_B can be made using Eq. (16). We find $E_B - E_v(\text{GaSb}) = 125$ meV, which is a plausible value, according to theoretical calculations.[11] Note, however, that these calculations were made for a (110) interface.

A question that naturally arises here is whether our observed values of mobility are compatible with such an amount of ionized donors at the interfaces. A rigorous answer to this question lies in mobility calculations which, for this system, would have to include screening effects, nonparabolicity, and electron-hole scattering in the semimetallic state. There are no such theoretical results available at this moment.

CONCLUSION

The decrease of carrier concentrations with pressure in GaSb-InAs-GaSb heterostructures is interpretable as being due to a transfer of electrons into the valence band of GaSb and/or into unoccupied interface donor states. A simple model shows that the density of interface states necessary to explain our results is of the order of 10^{12} cm^{-2}eV^{-1} on each interface (assuming that these are identical), and that the band discontinuity Δ decreases at a rate of 67 meV/GPa. Our calculations indicate that nonparabolicity of the InAs conduction band has an important influence on the values of the carrier concentrations, and it is therefore necessary to take it into account in order to do quantitative comparison with the experimental results.

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