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Theoretical and experimental capacitance-voltage behavior of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ modulation-doped heterojunctions: Relation of conduction-band discontinuity to donor energy

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For the first time, we show that the capacitance-voltage behavior of modulation-doped heterojunctions may be accurately described by a first-principles theory that includes self-consistent quantum two-dimensional (2-D) electron subbands in the GaAs, numerical solution of Poisson's equation for band bending and space charge in the (Al,Ga)As, and series resistance in the 2-D channel and heterointerface. The excellent agreement found between the theory and measurements on selected high-quality $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ heterojunctions allows accurate determination of the maximum 2-D carrier concentration. From this, we find a strong relationship between the conduction-band discontinuity and donor binding energy, giving offsets of 76 and 66% of the direct gap discontinuity for binding energies of 66 and 30 meV, as derived from published data.

With the development of molecular beam epitaxy (MBE), abrupt III-V semiconductor heterojunctions have attracted much interest for device applications. Of these systems, the $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterojunction has been the most widely studied, primarily as a result of its application in the modulation-doped heterojunction field-effect transistor (MODFET).¹ In this regard, the (Al,Ga)As/GaAs conduction-band discontinuity²⁻¹⁴ and (Al,Ga)As donor energies^{15,16} play a major role in MODFET operation, and much work has been devoted to their determination. In this letter we describe a novel alternative measurement relating these quantities based on capacitance-voltage (C - V) profiling of $n^+ \text{-Al}_{0.3}\text{Ga}_{0.7}\text{As}/p^- \text{-GaAs}$ MODFET's. The method utilizes the excellent agreement between theory and experiment for C - V profiles of selected high-quality MODFET devices to yield the maximum transferred 2-D electron density, N_{sat} , without the use of possibly ambiguous magnetotransport measurements.¹⁷ The measured value of N_{sat} is related to the conduction-band discontinuity, ΔE_c , and found to be relatively insensitive to the uncertainties in device parameters but quite sensitive to the (Al,Ga)As donor binding energy. An offset ratio of the conduction band to the valence band of 76.24 ± 5 is found for an assumed donor energy of 66 meV (after Chand *et al.*¹⁵), but 66.34 ± 5 results for an effective energy of 30 meV (derived from Schubert and Ploog¹⁶).

The MODFET structure we discuss here consists of the following component layers: (1) an unintentionally doped, thick p -type GaAs buffer layer, (2) a thin undoped $\text{Al}_x\text{Ga}_{1-x}\text{As}$ spacer of thickness d_1 , (3) a doped n -type $\text{Al}_x\text{Ga}_{1-x}\text{As}$ of thickness $d - d_1$ and doping density N_d , and (4) a metal gate, characterized by a Schottky barrier height V_s . Picking z as the coordinate perpendicular to the layers with $-d < z < 0$ in the (Al,Ga)As and $z > 0$ in the GaAs, the electronic structure of the system is described by the usual self-consistent Schrödinger equation^{18,19}

$$-\frac{\hbar^2}{2m} \nabla^2 \zeta_i(z) + [-e\varphi(z) + V_c(z) + V_{xc}(z)] \zeta_i(z) = E_i \zeta_i(z) \quad (1)$$

where ζ_i is the subband wave function, $V_c(z) = \Delta E_c \theta(-z)$ describes the conduction-band discontinuity, V_{xc} is a local density functional exchange-correlation potential, and $\varphi(z)$ is the electrostatic potential given by the Poisson equation

$$-\nabla^2 \varphi(z) = \frac{4\pi e}{\epsilon} (n_d(z) - n_e(z) - n_c(z) - n_a(z) - \sum_i n_i \zeta_i^2(z)). \quad (2)$$

Here, $n_d(z)$ is the density of ionized donors in the (Al,Ga)As, $n_e(z)$ is the free-electron density in the (Al,Ga)As, $n_c(z)$ is the density of compensating acceptors [taken as $CN_d(z)$ for a compensation ratio C and doping profile $N_d(z)$], $n_a(z)$ is the density of ionized residual acceptors in the GaAs, and n_i is the sheet density of electrons in the i th subband. The overlap of subband electrons at the heterojunction and charges in the (Al,Ga)As is small,^{18,20} so we solve Eqs. (1) and (2) for the 2-D subbands at the heterointerface, ignoring n_d and n_e , finding the electric field at $z = 0$ by conservation of charge. We use a set of orthonormalized Fang-Howard variational wave functions²¹ and take

$$n_i = (mkT/\pi\hbar^2) \ln \{1 + \exp[(E_f - E_i)/kT]\}, \quad (3)$$

where E_f is the Fermi energy and the other symbols have their usual meaning. Having found the subband energies E_i and occupancies n_i for a given Fermi energy, we solve the Poisson equation (2) numerically for $z < 0$, using $n_d(z)$

$$= \frac{N_d(z)}{1 + 2[\exp(E_s/kT) + \exp(E_d/kT)] \exp[(E_f - \varphi)/kT]}, \quad (4)$$

$$n_e(z) = N_{\text{dos}} \exp[(E_f - \varphi)/kT], \quad (5)$$

where E_s and E_d are shallow and deep levels of a single donor,¹⁵ and N_{dos} is the density of states for the Γ , X , and L minima in the (Al,Ga)As.²² The gate voltage corresponding to a given E_f is then given by $V_g = E_f + V_s + e\varphi(-d)$. The capacitances of the subband electrons, (Al,Ga)As donors and free electrons, and acceptors in the GaAs are given by

FIG. 1. MODFET capacitance vs gate bias. The theoretical C - V response of a $400 \times 50 \mu\text{m}^2$ gate size FET with $N_d = 2.8 \times 10^{18} \text{ cm}^{-3}$, $d = 367 \text{ \AA}$, and $d_1 = 150 \text{ \AA}$ is shown at 77 and 300 K. Curve (1) is the capacitance due to subband electrons; (2) is due to occupied donors in the (Al,Ga)As; (3) is due to free electrons in the (Al,Ga)As; (4) is due to acceptors in the GaAs buffer. Curve (5) is the total capacitance of (1)–(4).

the derivatives of the corresponding areal densities with respect to V_g . Typical results are shown in Fig. 1 for the case where V_{xc} and subband penetration into (Al,Ga)As are ignored.

The results shown in Fig. 1, computed as described above, neglect the effects of series resistance known to be important in high-frequency C - V measurements. In the gate-source C - V measurement described here, the current induced by the ac gate bias flows through the source contact (with contact resistance R_c), along the 2-D channel (with a finite resistivity $r_{2d} = L/\epsilon\mu n_s W$, for total subband areal density n_s , mobility μ , gate length L , and width W), and then into the (Al,Ga)As across the heterojunction (with an assumed constant specific resistance r_s). This assumes that the fully depleted GaAs buffer and low conductivity (Al,Ga)As layers are too resistive to support high-frequency current flow along the layers and that the applied dc biases are insufficient to cause significant leakage currents across the Schottky barrier. This model of ac current flow is incorporated into a distributed network using the computed C - V response and the resistive parameters described above, and the admittance is given by

$$A = \{ [A_0 \tanh(A_0 r_{2d})]^{-1} + R_c \}^{-1}, \quad (6)$$

where

$$A_0 = (1 + i) \left[\frac{\omega L W}{2 r_{2d}} \left(C_2 + \frac{C_3}{1 + i\omega C_3 r_s} \right) \right]^{1/2}. \quad (7)$$

Here, ω is the angular frequency, C_2 is the subband capacitance, and C_3 is the total (Al,Ga)As capacitance. Figure 2 shows the effects of this series resistance on the effective capacitance for the devices considered ($L = 50$ and $W = 400 \mu\text{m}$ at 1 MHz). Writing $A = G + i\omega C_{\text{eff}}$, the parallel conductance G is a measure of the distortion of the C - V response and assumes finite values when (1) in reverse bias, r_{2d} increases faster than C_2 decreases, and (2) in forward bias, the large value of C_3 leads to a significant ac voltage drop across the heterojunction resistance r_s .

A number of MODFET devices were characterized by

FIG. 2. Effective MODFET C - V response. The theoretical and experimental response of the MODFET described in Fig. 1 is shown, including series resistance effects at 1 MHz. Curve (1) is the "intrinsic" capacitance due to the subband electrons, donors, and free electrons in the (Al,Ga)As, without inclusion of series resistance. Curve (2) is the effective capacitance and curve (3) is the parallel conductance (measured in pF). (O) Experimental data for a selected MODFET.

C - V measurements at frequencies from 0.01 to 10 MHz and temperatures of 77 and 300 K. All devices were grown by MBE on semi-insulating substrates with an undoped GaAs buffer thickness of $1 \mu\text{m}$ followed by 380–500 $\text{\AA}$ of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$. The (Al,Ga)As consisted of an undoped spacer, ranging from 30 to 150 $\text{\AA}$, followed by Si doping concentrations of 1×10^{18} – $3 \times 10^{18} \text{ cm}^{-3}$. Gate recesses were chemically etched to a total (Al,Ga)As thickness of ~ 300 – $400 \text{ \AA}$ and had evaporated Al gates applied. At 77 K, a small fraction of the devices measured clearly exhibited the "double step" C - V profile shown in Fig. 2. The C - V response of these devices at 77 and 300 K was fit to the theory, assuming a Schottky barrier of $V_s = 0.9 \text{ eV}$, an Al mole fraction of $x = 0.3$, the specified spacer width, and a deep donor energy of $E_d = 66 \text{ meV}$. The series resistance parameters R_c and channel mobility were inferred from I - V and magnetotransport measurements. The three remaining free material parameters, total (Al,Ga)As thickness d , donor density N_d , and band offset ΔE_c , were varied to achieve the best fit in the region of the first step (due primarily to charge control of the 2-D electrons). The value of the heterojunction specific resistance r_s was chosen to give the best fit at large forward bias, where the response is due primarily to charge control of the (Al,Ga)As donors. As the C - V response in the region of the first step exhibits a definite onset, width, and height, the best fit yielded reasonably unambiguous values of d , N_d , and ΔE_c . In all cases, the determined values of these parameters satisfied the physical constraints: (1) ΔE_c constant for all samples, (2) d less than the metallurgical thickness of the (Al,Ga)As and independent of temperature, and (3) N_d constant at 300 K for all devices from the same wafer and in agreement with the approximate values determined from growth fluxes and forward-bias C - V measurements. The agreement between theory and experiment is generally excellent, with two exceptions. The deviation of the 300 K C - V response in forward bias from the predicted behavior is probably due to the assumption of a constant value of r_s , which is

FIG. 3. Relation between the conduction-band discontinuity and $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ deep donor energy as determined from the maximum 2-D carrier concentration N_{sat} for several MODFET's. The conduction-band offset ΔE_c is measured with respect to the total band-gap discontinuity ΔE_g . (●) From MODFET's with 150-Å spacers; (▲) for a 30-Å spacer. The difference between the curves is attributable to experimental errors and uncertainty in the spacer thickness.

strictly applicable only when the overlap of charge control in the subbands and (Al,Ga)As is negligible. The broadening of the measured C - V response compared to the theory was seen to a greater or lesser degree in all devices and is almost certainly due to fabrication nonuniformities in the (Al,Ga)As thickness d . The amount of deviation shown in Fig. 2 can be accounted for by a long-range variation in d of only ± 5 –10 Å. The lack of clear “double-step” behavior seen in many devices could easily be explained by somewhat larger deviations in d . Although the values of the fitted parameters were consistent between samples and with other measurements, their exact value could be affected by the fixed parameters chosen or assumptions made. However, the excellent fit of the overall C - V response allows the unambiguous determination of the maximum 2-D electron density, N_{sat} , which is directly related to an integral of the C_2 portion of the C - V curve. Thus, any set of parameters that gives an equally good fit will yield the same value of N_{sat} (estimated at $\pm 10\%$).

The theoretical value expected for N_{sat} is most strongly affected by the band offsets and the relation of the Fermi energy to the subbands and the (Al,Ga)As conduction band.²³ The maximum 2-D electron concentration occurs when near-flatband conditions occur between the Schottky and heterojunction depletion regions in the (Al,Ga)As. In this region, the Fermi energy is primarily determined by the deep energy level of the highly compensated donors for $x \geq 0.22$. In the subbands, the Fermi energy is strongly affected by the subband energy levels. In Fig. 3 we show the relation between the donor energy E_d and the band offset ΔE_c from experimentally determined values of N_{sat} in MODFET's with 150- and 30-Å spacers. In Fig. 3, the subband energies used to calculate the charge transfer were taken from Stern and Das Sarma,¹⁹ who include the significant effects of 2-D electron penetration into the (Al,Ga)As spacer and a local exchange-correlation potential V_{xc} . The donor energy of 66 meV was taken from Chand *et al.*¹⁵ for doping densities near $2 \times 10^{18} \text{ cm}^{-3}$. For the three best devices, with widely varying spacer thicknesses of 150 and 30 Å, a band offset of 76:24 was found. Assuming uncertainties of donor concentration $N_d \pm 5 \times 10^{17} \text{ cm}^{-3}$, Al mole fraction $x \pm 2\%$, spacer thickness $d_1 \pm 10\%$, interface charge $< 3 \times 10^{10} \text{ cm}^{-2}$, and donor energy $E_d \pm 10 \text{ meV}$, the uncertainty in conduction-band offset is estimated to be $\pm 5\%$. If the interface charge density is larger than the as-

sumed value, the results will be systematically increased toward a larger offset. Using the Hall data of Schubert and Ploog,¹⁶ one finds significantly lower *effective* binding energies, estimated at 30 meV for an Al mole fraction of 0.3. With this energy, we find an offset ratio of $66:34 \pm 5$. Although Schubert and Ploog postulate a more complex model of donor incorporation, involving separate shallow and deep donors, the Fermi level in the (Al,Ga)As will not significantly differ for a single effective heavily compensated deep donor level derived from the same data.

In conclusion, we have found excellent agreement between theory and experiment for the C - V behavior of high-quality $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ MODFET's. The fit between theory and experiment allows the accurate determination of the maximum 2-D electron density which, in turn, relates the (Al,Ga)As/GaAs band offsets to the (Al,Ga)As donor binding energies. Offsets of 76:24 and $66:34 \pm 5$ were found for experimental donor energies of 66 and 30 meV. The conclusive determination of band offsets by this method is, at present, limited by disagreements between measurements of these donor energies.

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- ¹P. M. Solomon and H. Morkoç, IEEE Trans. Electron Devices ED-31, 1015 (1984).
- ²R. Dingle, W. Weigmann, and C. H. Henry, Phys. Rev. Lett. 33, 827 (1974); R. Dingle, in *Festkörperprobleme*, edited by H. J. Queisser, Vol. 15 of *Advances in Solid State Physics* (Pergamon/Vieweg, Braunschweig, 1975), pp. 21–48.
- ³R. C. Miller, A. C. Gossard, D. A. Kleinman, and O. Munteanu, Phys. Rev. B 29, 3740 (1984).
- ⁴R. C. Miller, D. A. Kleinman, and A. C. Gossard, Phys. Rev. B 29, 7085 (1984).
- ⁵C. M. Wu and E. S. Yang, J. Appl. Phys. 51, 2261 (1980).
- ⁶A. C. Gossard, W. Brown, C. L. Allyn, and W. Wiegman, J. Vac. Sci. Technol. 20, 694 (1982).
- ⁷T. W. Hickmott, P. M. Solomon, R. Fischer, and H. Morkoç (unpublished).
- ⁸J. Batey, S. L. Wright, and D. J. DiMaria, J. Appl. Phys. 57, 484 (1985).
- ⁹D. Arnold, A. Ketterson, T. Henderson, J. Klem, and H. Morkoç, Appl. Phys. Lett. 45, 1237 (1984).
- ¹⁰W. I. Wang, E. E. Mendez, and F. Stern, Appl. Phys. Lett. 45, 639 (1984).
- ¹¹H. Kroemer, Wu-Yi Chien, J. S. Harris, Jr., and D. D. Edwall, Appl. Phys. Lett. 36, 295 (1980).
- ¹²R. People, K. W. Wecht, K. Alavi, and A. Y. Cho, Appl. Phys. Lett. 43, 118 (1983).
- ¹³H. Okumura, S. Misawa, S. Yosida, and S. Gonda, Appl. Phys. Lett. 46, 377 (1985).
- ¹⁴Herbert Kroemer, Appl. Phys. Lett. 46, 377 (1985).
- ¹⁵Naresh Chand, Tim Henderson, John Klem, W. Ted Masselink, Russ Fischer, Yia-Chung Chang, and Hadis Morkoç, Phys. Rev. B 30, 4481 (1984).
- ¹⁶E. F. Schubert and K. Ploog, Phys. Rev. B 30, 7021 (1984).
- ¹⁷E. F. Schubert and K. Ploog, Appl. Phys. A 33, 63 (1984).
- ¹⁸B. Vinter, Appl. Phys. Lett. 44, 307 (1984).
- ¹⁹Frank Stern and Sankar Das Sarma, Phys. Rev. B 30, 840 (1984).
- ²⁰George B. Norris, D. C. Look, W. Kopp, J. Klem, and H. Morkoç, J. Vac. Sci. Technol. B 2, 797 (1985).
- ²¹S. Das Sarma, R. K. Kalia, M. Nakayama, and J. J. Quinn, Phys. Rev. B 19, 6377 (1979).
- ²²H. C. Casey and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978).
- ²³Frank Stern, Appl. Phys. Lett. 43, 974 (1983).