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Effect of nonequilibrium deep donors in heterostructure modeling

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The deep donors (DX centers) which supply carriers in many GaAs-$Al_xGa_{1-x}As$ heterostructures are known to be metastable at low temperatures, maintaining a nonequilibrium state because of a microscopic barrier to recombination if ionized. Earlier modeling by three of us [Kumar, Laux, and Stern, Phys. Rev. B **42**, 5166 (1990)] incorrectly assumed the donors in the $Al_xGa_{1-x}As$ to be in equilibrium with the electrons in the GaAs channel. We present data on the threshold voltage of heterostructures cooled under bias and results of calculations which assume that the deep donor charge is locked at the value attained at 100 K when the sample is cooled with a bias voltage applied. The revised calculations account for part of the discrepancy between the calculated threshold voltage for the quantum dot structure used in experiments by Hansen *et al.* [Phys. Rev. Lett. **62**, 2168 (1989)] and the observed value. Part of the remaining discrepancy may be due to processing damage.

I. INTRODUCTION

Electrons are commonly introduced in GaAs-$Al_xGa_{1-x}As$ heterostructures by adding donors to the barrier material, usually with an undoped spacer layer separating the doped region from the GaAs region in which the carriers are found. Such donors, often called DX centers, are known to be metastable. If they are ionized, they do not return to the ground state at low temperatures because of a microscopic barrier that inhibits recombination. This field has a vast literature, and we refer only to a few articles that summarize relevant work.[1-3] If the donor doping density exceeds the density required to supply carriers to the channel and to compensate the charge associated with surface states, the remaining donors will be neutral.[4]

The density of electrons in the conducting channel is modulated by the gate voltage applied in an actual device structure, and therefore the charge on the deep donors might be expected to change with gate voltage if the donors were in equilibrium with the channel, as assumed in an earlier calculation by some of us.[5] Because of the nonequilibrium behavior of the deep donors, a more realistic model would fix the charge on the deep donors at the value attained at the temperature where they go out of equilibrium, of order 100–150 K for the situation considered here. Gate voltage changes applied when the sample is held at lower temperatures have little or no effect on the deep donor charge. The result can be a dramatic dependence of the low-temperature threshold gate voltage on the gate voltage applied as the sample is cooled.[6,7]

In this paper we present experimental results on a particular heterostructure sample to show the effect of cooling under different gate voltages on the threshold voltage for the appearance of charge in the channel. The measurements were taken both on the patterned quantum dot samples previously studied by Hansen *et al.*[8] (see also Smith *et al.*[9]) and on unpatterned control samples made from the same heterostructure material. We also present modeling results to show the effect of the nonequilibrium nature of the deep donors on electron confinement in the quantum dot.

II. THRESHOLD VOLTAGE FOR SAMPLES COOLED UNDER BIAS

The GaAs-$Al_{0.4}Ga_{0.6}As$ heterostructure material employed in these measurements is the same as used in earlier experiments[8,9] and simulations.[5] It is based on an n-type GaAs substrate layer with a net ionized donor concentration of 10^{18} cm^{-3}, an 80-nm layer of undoped GaAs (a background acceptor concentration of 10^{14} cm^{-3} is assumed), a 20-nm layer of undoped $Al_{0.4}Ga_{0.6}As$, a 20-nm layer of the same material with a donor concentration of 1.5×10^{18} cm^{-3}, and a 30-nm GaAs cap layer. On unpatterned samples a circular metal gate of 250-μm diameter was deposited directly on the cap layer. On patterned quantum dot samples the cap layer was etched away except in the central 300×300 nm^2 portion of a 500×500 nm^2 area, with the structure repeated on a square lattice over a 600×600 μm^2 field, which was subsequently covered with a metal gate. The samples were cooled from room temperature to $T=4.2$ K with a constant dc gate bias V_{gc} applied to the gate, $-0.3\leq V_{gc}\leq0.3$ V (higher values of $|V_{gc}|$ were avoided due to large leakage currents at room temperature). The gate voltage derivative dC/dV_g of the capacitance between the top metal gate and the substrate was then measured by superimposing a small signal $V_{ac}=10$ mV at a frequency $f=10$ kHz to the slowly swept gate bias and measuring the signal at $2f$ by lock-in detection. A typical dC/dV_g curve of an unpatterned sample cooled with the gate grounded ($V_{gc}=0$) is shown in the inset of Fig. 1, while the quantum dot sample traces were published previously.[8,9]

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As the samples were cooled with a constant, nonzero gate bias V_{gc}, the overall dC/dV_g line shape did not change. However, as shown in Fig. 1, the capacitance threshold (defined as the gate voltage at which dC/dV_g peaks) shifted with V_{gc}. When the gate bias during cooling was positive, $V_{gc} \geq 0$, the threshold shifted approximately linearly with V_{gc} in both patterned and unpatterned samples, showing a weak tendency to saturate for $V_{gc} \geq 0.3$ V. For V_{gc} negative during cooling, the threshold shift of the patterned sample saturated for $V_{gc} \leq -0.1$ V (see Fig. 1), while the unpatterned sample's threshold continued to shift weakly with V_{gc}. In the gate voltage range where the patterned and unpatterned sample thresholds track each other, there is an overall shift of $\simeq 0.15$ V between the two. Finally, the absolute magnitude of the peak in dC/dV_g (see inset of Fig. 1) normalized to unit area was larger in unpatterned samples than in patterned samples by a factor of ~ 150.

III. MODELING RESULTS

Our original calculations,[5] done in the Hartree approximation, assumed the donors to be in equilibrium with the channel. As noted above, a more realistic model assumes that the donor charge is "locked" when the sample is cooled through the temperature range 100–150 K. We have modified our modeling program to record the donor charge distribution at equilibrium at 100 K (calculated classically) with the gate voltage equal to the gate voltage V_{gc} applied during cool down, and have used this locked donor charge distribution in our quantum-mechanical self-consistent calculations at 4.2 K.

Shown in Fig. 1 are calculated threshold values for the patterned and unpatterned cases. The deep-donor density used in these calculations is 1×10^{18} cm^{-3}, smaller than the nominal density of 1.5×10^{18} cm^{-3}. The threshold voltage in the unpatterned cases is set at a channel electron density of 1×10^{10} cm^{-2}, and the threshold in the patterned case is set at $\frac{1}{6}$ electron per dot, consistent with the 500-nm repeat distance of the structure and with the observed difference in peak height.

The trend of the calculated curves follows that of the measured points, although the saturation effects are not as pronounced. The difference in calculated thresholds between the patterned and unpatterned samples is smaller than the observed difference, but that may result from the somewhat arbitrary choice of threshold for the calculated curves. The calculated curves assume a Schottky barrier height of 0.7 eV for the gate on GaAs and 1 eV on $Al_{0.4}Ga_{0.6}As$, and the measured and calculated voltage scales may be offset somewhat.

Figure 2 shows potential contours at the Fermi level in a plane near the peak of the induced electron charge in the GaAs channel, calculated using the original model and the revised model with locked charge. In each case the dot charge is fixed at seven electrons, but the gate

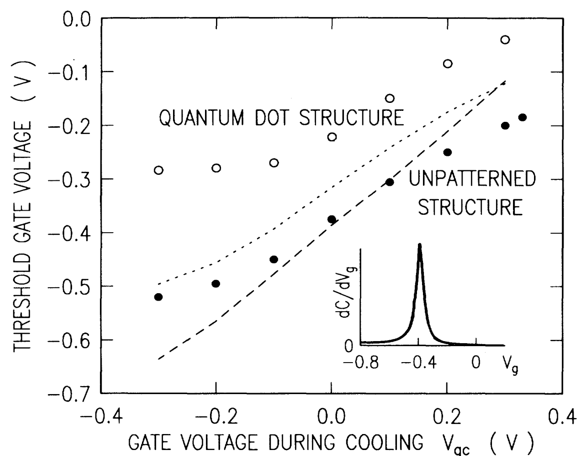

FIG. 1. Measured threshold voltage at 4.2 K for onset of channel charge in a heterostructure cooled with a gate voltage applied. The sample had an $Al_xGa_{1-x}As$ layer with AlAs fraction $x=0.4$ and nominal Si donor density of 1.5×10^{18} cm^{-3} separated from the GaAs channel by an undoped spacer layer 20 nm thick. The full circles are for unpatterned devices, and the open circles are for the quantum dot structures of Hansen *et al.* (Ref. 8). The dashed and dotted curves show the corresponding modeling results assuming the donors (with density taken to be 1×10^{18} cm^{-3} and effective thickness 23 nm) for the unpatterned and patterned structures, respectively, to be locked at the values attained at 100 K during cool down. The threshold densities for the unpatterned and patterned structures are 10^{10} electrons per cm^2 and $\frac{1}{6}$ electrons per dot, respectively. The corresponding calculated threshold voltages with the donors assumed to be in equilibrium with the channel electrons are -0.67 and -0.50 V, respectively. The inset shows a representative trace of the derivative of the capacitance with respect to gate voltage vs gate voltage. The measured gate voltage at the peak gives the ordinate for the plotted points.

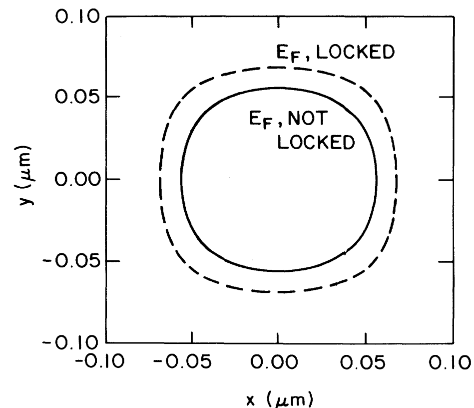

FIG. 2 Calculated contours showing the Fermi level in the plane 9.5 nm below the GaAs-$Al_xGa_{1-x}As$ interface, near the peak of the vertical electron density, for the quantum dot structure of Hansen *et al.* (Ref. 8). The dashed contour is for a gate voltage of -0.45 V when the deep donors are assumed to be locked in the charge state corresponding to zero gate voltage during cool down. The solid contour is for a gate voltage of -0.26 V when the deep donors are assumed to be in equilibrium with the channel electrons. The electron channel and the n^+ GaAs substrate are taken to be at ground throughout. Both cases correspond to a charge of seven electrons in the quantum dot.

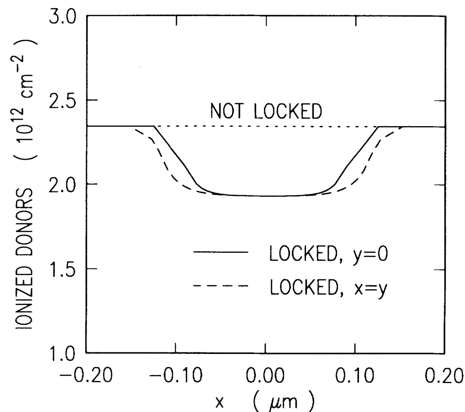

FIG. 3. Integrated sheet density of ionized donors, for the same conditions as in Fig. 2. The dotted curve, with all donors ionized, corresponds to donors in equilibrium with the channel electrons. The full and dashed curves correspond to donors locked at the charge they have at 100 K during cool down with zero gate voltage applied, and reflect horizontal and diagonal slices, respectively.

voltage is 0.19 V larger for the locked charge case because of the higher threshold voltage. Locking the charge leads to a larger dot and correspondingly larger gate-dot capacitance. Note that here, as in the earlier calculation, a small neck of charge connects the quantum dot to the n^+ substrate, leading to some arbitrariness in the magnitude of the charge on the dot. Figure 3 shows the lateral variation of integrated sheet charge on the deep donors for the two cases of Fig. 2. Locking the charge reduces the effect of the donors in screening the gate potential, and therefore results in a potential that more closely reflects the square shape of the overlying structure.

IV. DISCUSSION

The discrepancy between calculated and measured threshold voltage in our earlier calculation for quantum wires[10] and quantum dots[5] was attributed to the effect of processing damage. There is voluminous literature showing that certain kinds of patterning, including the reactive ion etching used to fabricate the samples used in the experiments of Refs. 8 and 9, introduce significant changes in transport and other properties.[11-14] The effects of processing damage are not amenable to simple modeling but presumably affect the samples considered here and need further investigation.

Although calibrations give information about impurity concentrations in relation to growth conditions, some effects such as compensation and impurity motion during and after sample growth can complicate the doping structure in a given sample. Thus, there is not always definitive information about the donor concentration and its spatial distribution, which is an additional unknown in modeling. Our results suggest that the net donor concentration in the samples considered here is somewhat less than the nominal value.

Despite these uncertainties, the results presented here show that the nonequilibrium behavior of deep donors is one source for the difference between calculated and measured threshold voltages in the samples considered here and presumably in other samples. Careful comparison between experiments and realistic models for patterned and unpatterned structures, perhaps also including the effect of persistent light-induced changes in carrier concentration, should make it possible to narrow the uncertainties in sample parameters and attain satisfactory agreement between models and experiments.

We have considered a particular doping structure here. The extent to which nonequilibrium effects enter in other samples depends strongly on the excess donor concentration.

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[1] P. M. Mooney, J. Appl. Phys. **67**, R1 (1990).

[2] P. M. Mooney and T. N. Theis, Comments Condens. Matter Phys. **16**, 167 (1992).

[3] D. V. Lang, in *Deep Centers in Semiconductors,* 2nd ed., edited by S. T. Pantelides (Gordon and Breach, Yverdon, 1992), pp. 591–641.

[4] There is good evidence (see, for example, Ref. 2) that deep donors in $Al_xGa_{1-x}As$ are "negative-*U*" centers, preferring to be either positively or negatively charged rather than neutral, but we ignore that aspect here since it complicates the discussion without changing the qualitative aspects of the threshold behavior considered here.

[5] A. Kumar, S. E. Laux, and F. Stern, Phys. Rev. B **42**, 5166 (1990).

[6] P. M. Mooney, P. M. Solomon, and T. N. Theis, in *Gallium Arsenide and Related Compounds 1984,* edited by B. de Cremoux, IOP Conf. Ser. No. 74 (Institute of Physics, and Physical Society, London, 1985), p. 617; P. M. Mooney, N. S. Caswell, and S. L. Wright, J. Appl. Phys. **62**, 4786 (1987); T. N. Theis and B. D. Parker, Appl. Surf. Sci. **30**, 52 (1991).

[7] C. Ghezzi, E. Gombia, and R. Mosca, Semicond. Sci. Technol. **6**, B31 (1991).

[8] W. Hansen, T. P. Smith III, K. Y. Lee, J. A. Brum, C. Knoedler, D. Kern, and J. M. Hong, Phys. Rev. Lett. **62**, 2168 (1989).

[9] T. P. Smith III, K. Y. Lee, C. M. Knoedler, J. M. Hong, and D. P. Kern, Phys. Rev. B **38**, 2172 (1988).

[10] S. E. Laux, D. J. Frank, and F. Stern, Surf. Sci. **196**, 101 (1988).

[11] H. F. Wong, D. L. Green, T. Y. Liu, D. G. Lishan, M. Bellis, E. L. Hu, P. M. Petroff, P. O. Holtz, and J. L. Merz, J. Vac. Sci. Technol. B **6**, 1906 (1988).

[12]W. Beinstingl, R. Christanell, J. Smoliner, C. Wirner, E. Gornik, G. Weimann, and W. Schlapp, Appl. Phys. Lett. **57**, 177 (1990).

[13]D. Lootens, P. Van Daele, P. Demeester, and P. Clauws, J. Appl. Phys. **70**, 221 (1991).

[14]M. Rahman, N. P. Johnson, M. A. Foad, A. R. Long, M. C. Holland, and C. D. W. Wilkinson, Appl. Phys. Lett. **61**, 2335 (1992).