Spatial localization of impurities in δ-doped GaAs

E. F. Schubert,[a] J. B. Stark,[b] B. Ullrich,[c] and J. E. Cunningham
AT&T Bell Laboratories, Holmdel, New Jersey 07733

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Capacitance-voltage profiles on δ-doped GaAs grown by molecular beam epitaxy reveal extremely narrow widths of $\lesssim 40$ Å at room temperature. Subband structure and capacitance-voltage (C-V) profiles of δ-doped GaAs are calculated self-consistently. Experimental C-V profiles agree with self-consistent results, only if we assume that Si impurities are localized on the length scale of the lattice constant in the host GaAs zinc-blende lattice.

Spatial localization in a single monolayer of a semiconductor crystal[1-3] represents the ultimate physical limit of impurity distributions. The Dirac–delta function has been used[2,3] to describe such doping profiles. A schematic sketch of a δ-doped semiconductor is shown in Fig. 1. Si impurities are localized in a Ga plane of GaAs within the length scale of the lattice constant a_0. Even though monolayer distribution has been implicitly assumed in several publications,[1-4] there has been no experimental proof for such a narrow distribution. The important question of diffusion in Si planar or δ-doped GaAs has been first addressed by Lee *et al.*,[5] who concluded that diffusion over 126 Å occurs at least under their specific crystal growth conditions. Zrenner *et al.*[6] concluded that segregation over a length of 195 Å occurs in highly δ-doped GaAs. It is the purpose of this letter to demonstrate that a monolayer distribution of Si impurities can be realized under appropriate crystal growth conditions. We will show by capacitance-voltage profiling that neither diffusion nor segregation is relevant in our δ-doped GaAs samples, i.e., we investigate a structural characteristic of a semiconductor by means of its electronic properties.

Capacitance-voltage (C-V) profiling is a versatile means to spatially resolve doping profiles in semiconductors. This method, though introduced for homogeneously doped semiconductors, can also be used for quantum-mechanical systems such as δ-doped semiconductors. The interpretation of C-V measurements on δ-doped semiconductors requires, however, accurate knowledge of the electronic subband structure, which can be obtained by a self-consistent solution of Schrödinger's and Poisson's equations.

The self-consistently calculated subband structure of δ-doped GaAs is shown in Fig. 2. In this calculation we use a parabolic conduction-band dispersion, a dopant concentration of $N_D^{2D} = 5\times 10^{12}$ cm^{-2} localized within $dx = 2$ Å at 600 Å below a positively biased metal-semiconductor (Schottky) contact. The background doping is n-type, with concentration $N_D = 10^{14}$ cm^{-3}. The self-consistent calculation yields four occupied subbands of energy $E_0 - E_3$. The wave functions are normalized so that the probability densities $\psi(x)\psi^*(x)$ shown in Fig. 2 are indicative of the population of the four eigenvalues. The parabolic dispersion relation used here results in only minor changes of subband energies of $< 10\%$[6] as compared to a nonparabolic dispersion relation. Many-body effects, which have not been taken into account, are negligible in the density regime studied here, due to a higher average kinetic carrier energy than the average interaction energy.[7]

Theoretical C-V profiles are obtained from a series of self-consistent calculations under different bias conditions. Each self-consistent calculation performed for a specific voltage yields a two-dimensional electron gas concentration n_{2DEG}. The capacitance is obtained according to $C = d(qn_{2DEG})/dV$. Finally, the C-V profile is calculated following well-known equations. Two theoretical C-V profiles are shown in Fig. 3 for a diffusion length $dx = 2$ Å and for $dx = 50$ Å. For the sake of simplicity we use a constant top hat instead of a Gaussian impurity distribution. Both distributions yield very similar results if the width of the constant top-hat distribution is taken to be twice the standard deviation of the Gaussian distribution. Figure 3 reveals that C-V profiles depend sensitively on the δ-doped layer width, broadening from 41 ± 4 Å to 75 ± 5 Å as dx is changed from 2 to 50 Å. In addition the maximum concentration decreases from 1.32×10^{19} to 8.5×10^{18} cm^{-3} for $dx = 2$ and 50 Å, respectively. Thus, C-V profiling is well suited to study diffusion on the Å scale. In the following, we will describe experimental procedures, present experimental results, and compare them with theoretical calculations.

The δ-doped GaAs samples are grown by gas-source molecular beam epitaxy (Vacuum generator V80 system). A two-dimensional Si dopant concentration of 10^{12} cm$^{-2} \leqslant N_D^{2D} \leqslant 8\times 10^{12}$ cm^{-2} located 400 Å below the surface is used. The epitaxial layers with a total thickness of 1 μm are grown on heavily doped n^+-type GaAs substrates. The unintentionally doped buffer layer has n-type conductivity with an impurity concentration of $N_D + N_A = 5\times 10^{13}$ cm^{-3}

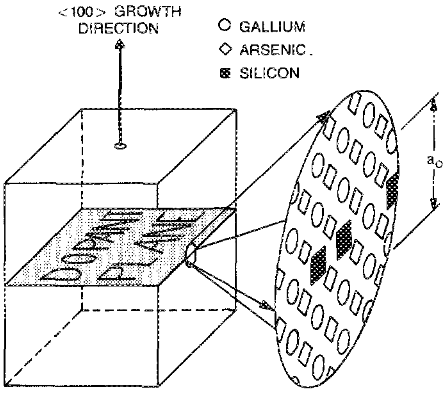

FIG. 1. Schematic illustration of δ-doped GaAs. Si impurities are localized in a gallium plane of the zinc-blende lattice.

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[a] AT&T Bell Laboratories, Murray Hill, NJ 07974.
[b] Massachusetts Institute of Technology, Cambridge, MA 02139.
[c] Max-Planck-Institute for Solid State Research, Stuttgart, FRG.

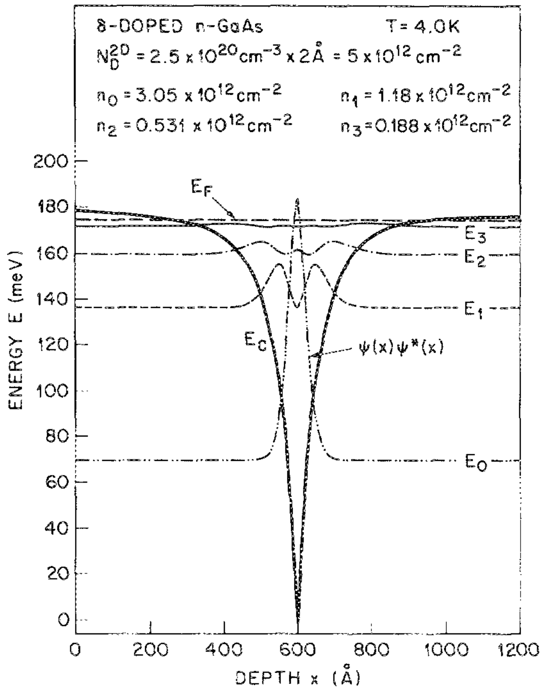

FIG. 2. Self-consistently calculated subband structure of δ-doped GaAs with a two-dimensional electron gas concentration of $N_D^{2D} = 5 \times 10^{12}$ cm^{-2}.

and a peak mobility of 270 000 cm^2/V s at 40 K. The substrate temperature used for growth is ⩽550 °C. Circular Ti/Au (500 Å/1500 Å) contacts (Φ 500 μm) are evaporated through a shadow mask in a separate vacuum system immediately after the samples are taken out of the growth system. The *C-V* curves are measured with a Hewlett–Packard 4194A impedance/gain-phase analyzer. A phase angle close to 90° is obtained during the *C-V* measurements indicating the dominating capacitance of the sample. Residual parasitics are compensated carefully. A frequency of 1 MHz is used for the measurements. Additional current-voltage measurements yield an excellent ideality factor of 1.04 and a breakdown voltage of − 5 V in reverse bias.

Experimental *C-V* profiles on δ-doped GaAs are shown in Fig. 4 on a (a) linear and (b) logarithmic ordinate. The maximum *C-V* peak occurs at a depth of 388 Å which compares favorably with the anticipated depth of 400 Å. The profiles have a peak concentration of 1.19×10^{19} cm^{-3}. The full width at half-maximum of these profiles is 40 Å which are the narrowest *C-V* profiles reported for any semiconductor structure with an *n*-type background concentration.

The *C-V* profile is shown on a magnified abscissa scale in Fig. 5. The free-electron concentration of the two-dimensional electron gas is obtained by integration of the *C-V* profile between appropriate voltages, i.e., $-\infty \leqslant V \leqslant 0$ V, as shown by the shaded area in Fig. 5, yielding a free-carrier concentration of 5.4×10^{12} cm^{-2}. The total dopant concentration is obtained by adding the concentration of carriers localized in surface states, N_{ss}, to the free-electron concen-

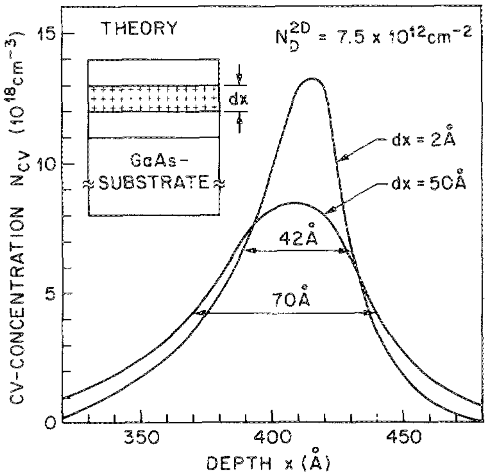

FIG. 3. Self-consistently calculated *C-V* profiles for δ-doped GaAs with no diffusion ($dx = 2$ Å) and a diffusion over $dx = 50$ Å. The inset shows the diffusion of donors over dx.

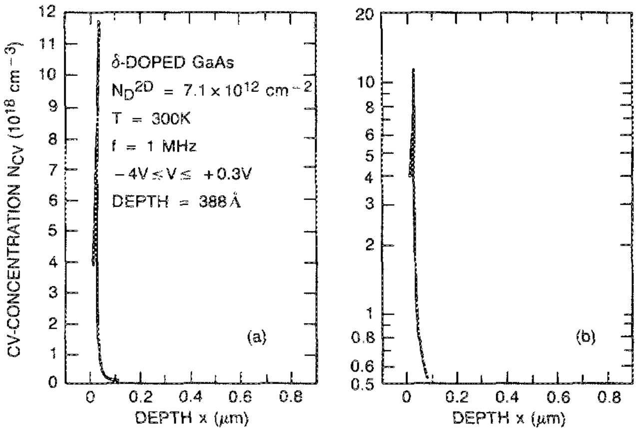

FIG. 4. Experimental *C-V* profiles of δ-doped GaAs on a (a) linear and (b) logarithmic ordinate scale. The full width at half-maximum of the profiles is 40 Å. The abscissa of 1 μm coincides with the entire thickness of the epitaxial layer.

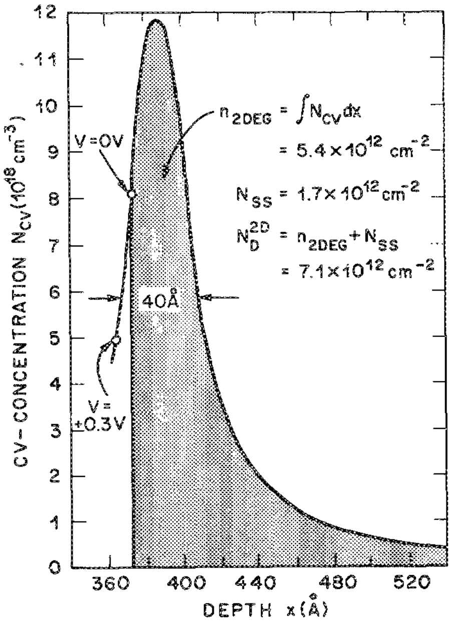

FIG. 5. Experimental *C-V* profile of a δ-doped GaAs sample. Integration of the profile (shaded area) yields a free-carrier concentration of 5.4×10^{12} cm^{-2} and a total doping concentration of 7.1×10^{12} cm^{-2}.

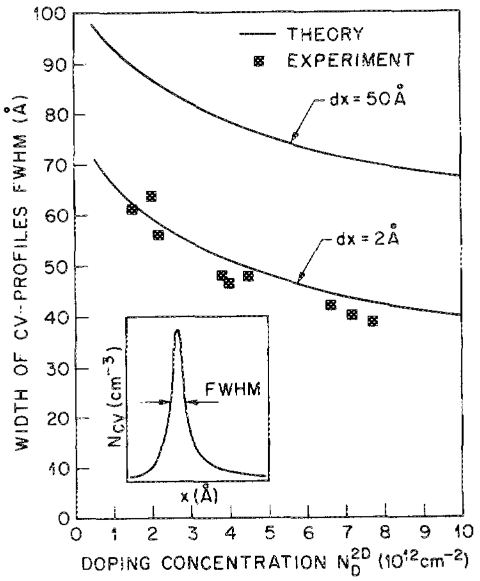

FIG. 6. Comparison of theoretical (solid line) and experimental (dark squares) widths of C-V profiles on δ-doped GaAs. Good agreement is obtained, only if we exclude diffusion.

tration.[8] This yields a total dopant concentration of $N_D^{2D} = 7.1\times10^{12}$ cm^{-2}, which is rather high. The high doping concentration in our samples is favorable to study diffusion effects.

A comparison of experimental C-V profile widths with theoretical C-V profile widths is shown in Fig. 6. The theoretical C-V profile widths are calculated (i) in the absence of diffusion ($dx = 2$ Å) and (ii) for diffusion over 50 Å. A comparison of the theoretical solid curves with experimental data (dark squares) shows that a good agreement is obtained, only if we assume absence of diffusion over more than two lattice constants. The fit of measured and calculated data is typically within 5% for both C-V profile width and C-V profile peak concentration. This comparison demonstrates that diffusion or segregation is unimportant in the samples used for this study. A localization of impurities on the length scale of the lattice constant is therefore concluded for concentrations 1×10^{12} cm$^{-2} \leqslant N_D^{2D} \leqslant 8\times10^{12}$ cm^{-2}.

Even though diffusion does not play an important role in the samples used for the present study, we do observe a broadening of C-V profiles to widths exceeding 100 Å, if the samples (i) are subject to rapid thermal annealing or (ii) grown under high growth temperatures, e.g., 650 °C. These findings may explain the observation of diffusion and segregation by Lee *et al.*[5] and Zrenner *et al.*[6]

In conclusion, we have investigated spatial localization of impurities in δ-doped GaAs. This structural characteristic was studied by means of electronic properties, i.e., capacitance-voltage (C-V) measurements. Comparison of self-consistently calculated C-V profiles with our experimental data yields a good agreement, only if we assume a localization of impurities on the length scale of the lattice constant. The comparison allows us to exclude diffusion of Si impurities in δ-doped GaAs over more than two lattice constants.

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