Extraction of parameters of surface states from experimental test structures

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Abstract

We present a procedure for extracting the parameters of a simple model for localized states at the exposed surfaces of GaAs/AlGaAs heterostructures. Such a procedure is based on a comparison between experimental data on test structures and results from the solution of the Poisson–Schrödinger equation in the growth direction of the heterostructure. We show that a model of surface states based on just two parameters is sufficient for obtaining good agreement with experiments and significant improvement with respect to the assumption of Fermi level pinning. In addition, the procedure proposed allows the extraction of the donor concentration in the doped layer and the unintentional doping in the substrate.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The surface-to-volume ratio of mesoscopic and nanoelectronics devices increases as geometries are scaled down, so that device characteristics are increasingly affected by the properties of the surface. This is a relevant issue in all fields of nanotechnology, since the mechanical, thermal and electrical properties of nanoscale structures depend on surface characteristics, which, in turn, depend on the fabrication process and may vary with time as a consequence, for example, of contamination or oxidation.

In this paper, we want to address the characterization of states at the exposed surfaces of AlGaAs/GaAs heterostructures. Such states strongly affect the electrical properties of mesoscopic devices defined by split gates on a shallow two-dimensional electron gas (2DEG) obtained at the AlGaAs/GaAs heterointerface.

The accurate simulation of such devices certainly requires that surface states be properly taken into account through simple and effective models, whose parameters may be experimentally determined.

We consider two models originally used for the treatment of states at the metal–semiconductor surface [1], and propose a procedure for extracting the model parameters from measurements of electron density in the 2DEG on purposely fabricated test structures and from numerical simulations of the potential profile in the vertical direction. We show that a model based on just two parameters is very effective in reproducing the experimental results. The procedure also allows us to determine the unintentional doping in the substrate and the donor concentration in the doped layer, which are usually known with limited accuracy.

2. Models of surface states

A commonly adopted approximation to take into account surface states is Fermi level pinning, which consists of considering the Fermi level at the surface 'pinned' at a given level in the bandgap. This assumption was typically made for treating states at the interface of metal–semiconductor contacts [1], where the level at which the Fermi energy is pinned can be extracted from the experimental I–V characteristic of the resulting Schottky diode. It has been very often applied to the exposed surface of heterostructures, even if it has obvious limitations, such as the discontinuity of the potential energy at the edges of the metal gates evaporated on the exposed surface [2].

Another possible approach is to impose Neumann boundary conditions at the surface [3, 4]. In this case the gradient of the potential in the direction orthogonal to the surface $\vec{n}$ is assumed to be

$$\epsilon \frac{\partial \phi}{\partial \vec{n}}\bigg|_{surf} = Q_{surf}, \tag{1}$$

where Q_{surf} is the charge at the surface and ϵ is the dielectric constant of the semiconductor. The charge at the interface is 'frozen' and cannot move in response to an electric field. The boundary conditions for the Poisson equation are determined by the voltages applied to the contacts. Unfortunately this approximation is only valid if the exposed surface is large and regular [5] and this cannot be true in the case of nanostructures.

Chen and Porod [6] proposed an alternative method consisting of broadening the simulation domain. The electrostatic problem is solved in a domain containing both the dielectric (air) and the semiconductor: the Laplace equation is solved in the former and the Poisson equation in the latter. The potential distribution at the air–semiconductor interface is obtained by coupling the solutions of the two equations. Davies and Larkin [7–9] have shown that the shape of the potential in a GaAs/AlGaAs heterostructure depends on the boundary conditions on the GaAs exposed to air between the metallic gates. They compare two assumptions: the Fermi level pinning and the 'frozen' charge approximation. They also assume that for a generic semiconductor the large dielectric constant makes it possible to neglect the electric field outside the structure. They found that the model provides reasonable predictions for devices that operate at low temperature. In [10] the same two models have been compared in the simulation of quantum point contacts (QPCs): the 'frozen' charge model allows us to achieve better agreement with the experiments, though not completely satisfactory.

Q.2

Here, we want to consider a slightly more complex model, based on two parameters, which reduces to Fermi level pinning as a particular case. Such a model is rather common in the context of metal–semiconductor contacts [1].

Figure 1 shows the energy band diagram at the exposed surface of a generic n-type semiconductor. The two parameters are the effective work function Φ^* and a uniform density per unit area per unit energy D_s: $q\Phi^*$ represents the difference between the vacuum level E_0 and the Fermi level E_F when no charge is present at the surface. All the energy states that are below $E_0 - q\Phi^*$ behave like donors and all surface states above $E_0 - q\Phi^*$ like acceptors. Then $q\Phi_0 = E_g + q\chi - q\Phi^*$ represents the energy range of donor states (q is the electron charge, E_g the energy gap, and χ the electron affinity). The charge per unit area Q_s at the air–semiconductor interface is given by the expression

$$Q_s = -qD_s\,[E_F - (E_0 - q\Phi^*)]. \tag{2}$$

If $D_s \to \infty$ we have Fermi level pinning at the surface, that is the Fermi level of the semiconductor is pinned at the value $E_0 - q\Phi^*$ imposed by the surface states, and $q\Phi^*$ really behaves as a work function (in this case we have $\Phi_m = \Phi^*$). For typical values of D_s the difference between the vacuum energy level and the Fermi level at the surface differs from E_F by fractions of the bandgap; for this reason $q\Phi^*$ is an effective work function.

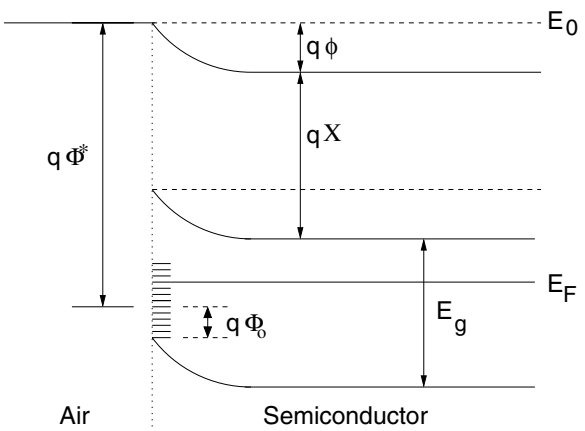

Figure 1. Typical band profile at the exposed semiconductor surface. $q\Phi_0$ represents the level below which all the interface states must be filled to have a neutral surface. $q\Phi^*$ is the effective work function and E_F is the Fermi level.

3. Experiment

Five different samples have been grown by molecular beam epitaxy on undoped GaAs wafers at a temperature of 590 °C starting with a 2 μm thick GaAs buffer followed by a layer sequence, which is schematically depicted in the left part of figure 2. Different $Al_{0.2}Ga_{0.8}As$ spacers with thicknesses ranging from 20 to 60 nm have been realized. The thicknesses have been changed in steps of 10 nm. Each spacer was covered by 40 nm thick Si-doped $Al_{0.2}Ga_{0.8}As$ with a doping concentration of 2×10^{18} cm^{-3}. The samples were finished by an undoped 10 nm thick GaAs cap layer. In addition we have performed wet etching to remove the upper surface layers of the sample with the 20 nm thick spacer [11]. The etching rate was 3 nm s^{-1}. We have removed up to 38 nm from the initial sample surface in steps of six etching processes. A scheme of the resulting samples is shown in the right part of figure 2. We determined the electron concentration of all samples described above by Hall measurements at 4.2 K in the dark [12].

4. Simulation

The band and charge density profiles in the heterostructures are obtained by solving the Poisson and Schrödinger equations self-consistently in the vertical direction. The Poisson equation in the structure reads

$$\nabla \cdot [\epsilon(x)\nabla\phi(x)] = -\rho(x), \tag{3}$$

where ϕ is the potential, $\epsilon(x)$ is the dielectric constant and $\rho(x)$ is the charge density, obtained by summing the contribution of holes, electrons, ionized dopants and surface charge. The Poisson equation is initially solved by assuming a semiclassical expression for electrons and holes. However, electrons in the 2DEG are strongly confined and the density of states must be computed by solving the Schrödinger equation. The solution of the Poisson equation is therefore substituted in the conduction band term of the Schrödinger equation

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left[\frac{1}{m_x(x)}\frac{\partial\psi(x)}{\partial x}\right] + E_C(x)\psi(x) = E\psi(x) \tag{4}$$

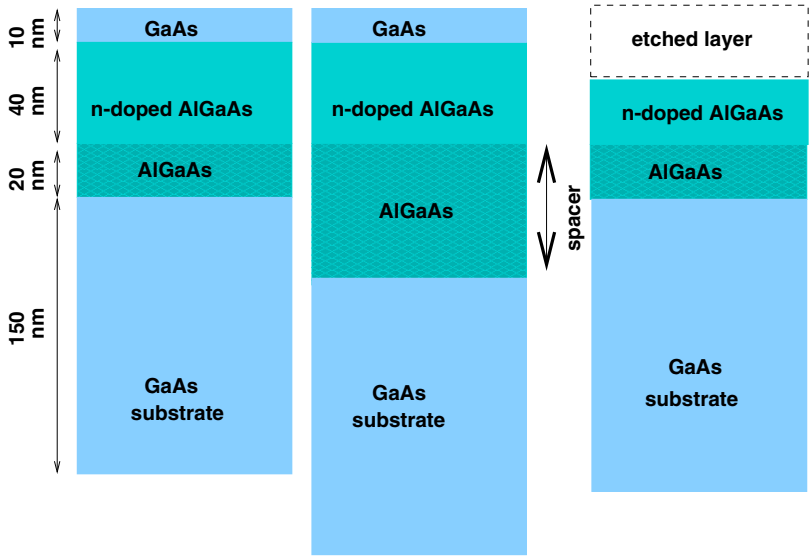

Figure 2. The first set of test structures consists of heterostructures differing only by the spacer layer thickness. The donor concentration of doped AlGaAs is of the order of 10^{24} m^{-3}, while the substrate has unintentional acceptor doping. The second set of test structures consists of a single heterostructure with a 20 nm spacer layer, progressively etched.

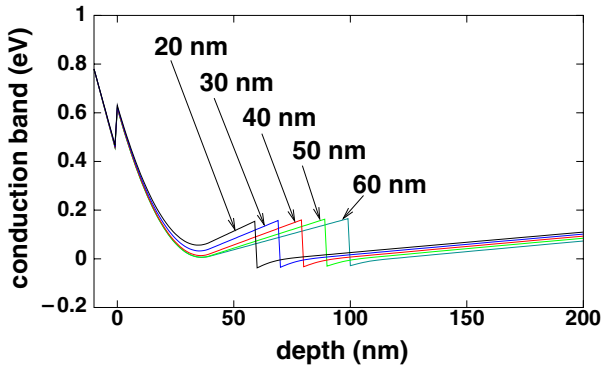

Figure 3. Theoretical conduction band profiles for different spacer layer thicknesses varying from 20 to 60 nm.

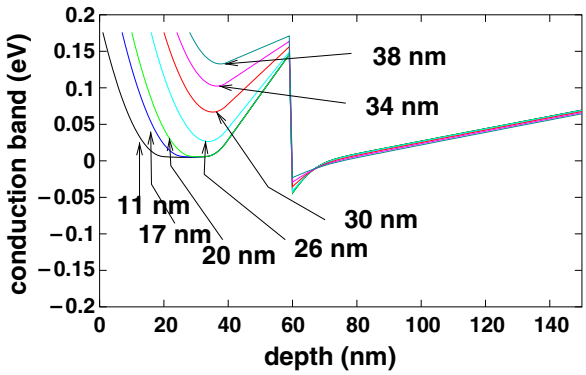

Figure 4. Theoretical conduction band profiles for different thickness of the etched layer varying from 11 to 38 nm.

in which $E_C(x)$ represents the conduction band energy, $m_x(x)$ is the effective mass in the confinement direction, and E is the eigenvalue corresponding to the eigenfunction $\psi(x)$. From the eigenfunctions and eigenvalues we deduce the numerical density of electrons $n(x)$ with the expression

$$n(x) = \frac{g}{\pi}\frac{2m_x K_B T}{\hbar^2}\sum_i |\psi_i(x)|^2 \ln\left[1+\exp\left(\frac{E_F - E_i}{k_B T}\right)\right] \tag{5}$$

where the sum is over all eigenvalues E_i and eigenfunctions ψ_i and g is the degeneracy factor (1 for GaAs). From equation (5) we calculate the new charge $\rho(x)$ and solve again equation (3). The cycle is repeated until two consecutive solutions have a difference smaller than a predefined value, in which case it is stopped. Figures 3 and 4 show the computed conduction bands for the test structures. In figure 3 the spacer thickness varies from 20 to 60 nm, in figure 4 the etch depth varies from 11 to 38 nm.

5. Extraction of the model parameters

In this section we present a procedure based on the measurements and the simulations described above to extract the value of quantities that have a significant impact on the electrical properties of the heterostructure. In particular, the value of the unintentional acceptor doping N_a in the GaAs substrate and the value of the active donor doping concentration N_d in the doped AlGaAs layer are usually not known with sufficient precision. In addition, we must determine the influence of the surface states through the value of the pair (Φ^*, D_s) in the case of the two-parameter model described in section 2 or of the work function Φ_m in the case of Fermi level pinning ($D_s \to \infty$). The electrical behaviour of devices defined on GaAs/AlGaAs heterostructures is very sensitive to all the above parameters.

In the test samples, progressively etched, the GaAs cap layer is completely removed, so that the material exposed to air is AlGaAs. In addition, etched structures have undergone an additional process step. This implies that the parameters of the surface states for the initial set of samples and for the etched samples are in general different. On the other hand, the values of N_a and N_d are common to all the test structures.

To devise a procedure for extracting the values of the mentioned parameters we would like to find relationships between a measurement on a particular sample and one unknown parameter.

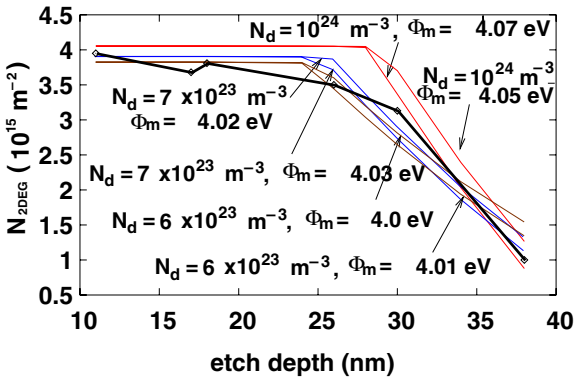

Figure 5. The best fits for the exposed AlGaAs with the Fermi level pinning approximation. Experiments are plotted by the thick curve. The thin curves are the simulations with $N_a = 3 \times 10^{20}$ m^{-3}, N_d varying from 6×10^{23} to 10^{24} m^{-3} and Φ_m from 4.01 to 4.09 eV.

Table 1. Sensitivities of N_{2DEG} to parameters in the approximation of Fermi level pinning, in the case of exposed GaAs (left column) and exposed AlGaAs (right column).

	60 nm spacer thickness	1 nm etch depth
$S^{N_a}_{N_{2DEG}}$	0.15	0.11
$S^{N_d}_{N_{2DEG}}$	3×10^{-5}	0.12
$S^{\Phi_m}_{N_{2DEG}}$	9×10^{-4}	2×10^{-3}

In order to do so we focus on the structure with just the cap layer removed (etch depth 11 nm), and on the structure with the thickest spacer layer (60 nm). As can be seen from figures 4 and 3, respectively, both structures have incomplete ionization of the donor layer. A varying charge in the donor layer can completely screen the electric field, so that the 2DEG in both cases is practically insensitive to the surface charge.

We have used our Poisson–Schrödinger solver to compute the sensitivity S^X_{2DEG} of the N_{2DEG} to the variation of the generic parameters X defined as

$$S^X_{2DEG} = \frac{\partial N_{2DEG}}{\partial X} \frac{X}{N_{2DEG}}.$$

In table 1 we show the sensitivities of N_{2DEG} to the three parameters required in the approximation of Fermi level pinning, computed for the structure with the 60 nm spacer in the case of exposed GaAs and the structure with the etch depth of 11 nm in the case of exposed AlGaAs. As can be seen, $S^{N_a}_{2DEG}$ is large in both cases, while $S^{N_d}_{2DEG}$ is large only for small etch depth and $S^{\Phi_m}_{2DEG}$ is always small. This means that for large spacer thickness N_{2DEG} depends mostly on N_a and little on N_d, D_s and Φ^*. We can therefore obtain N_a by fitting N_{2DEG} for the sample with the 60 nm spacer layer and then, once N_a is fixed, obtain N_d, since N_{2DEG} for small etch depths depends essentially only on N_d.

We find $N_a = 3 \times 10^{20}$ m^{-3} and $N_d = 6 \times 10^{24}$ m^{-3}. The third step consists of finding the value of Φ^* giving the best fit for samples with a thinner spacer layer, for exposed GaAs, and larger etch depth, for the exposed AlGaAs. We find $\Phi_m = 4.68$ eV for exposed GaAs, and $\Phi_m = 4$ eV for exposed AlGaAs.

In figure 5 the theoretical values of N_{2DEG} as a function of the etch depth are plotted for different values of the parameters

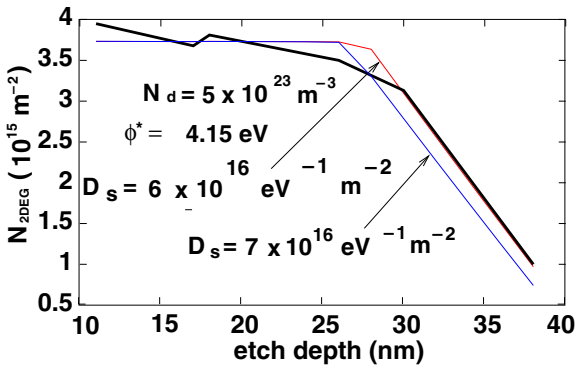

Figure 6. Sheet electron density as a function of the etch depth for the two-parameter model. Experiments are plotted with the thick curve, simulations are plotted with the thin curve with $N_a = 3 \times 10^{20}$ m^{-3} and $N_d = 5 \times 10^{23}$ m^{-3}. The best fit is for $\Phi^* = 4.15$ eV and $D_s = 6 \times 10^{16}$ eV^{-1} m^{-2}.

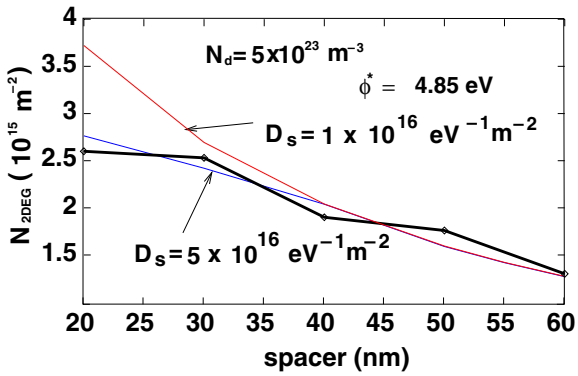

Figure 7. Sheet electron density as a function of the spacer thickness for the two-parameter model. Experiments are plotted with the thick curve, simulations are plotted with the thin curve with $N_a = 3 \times 10^{20}$ m^{-3} and $N_d = 5 \times 10^{23}$ m^{-3}. The best fit is for $\Phi^* = 4.85$ eV and $D_s = 5 \times 10^{16}$ eV^{-1} m^{-2}.

(thin curves), while experimental values are plotted with solid curves. Errors are smaller than 3 nm on the etch depth, and smaller than 1.5% on the electron concentrations. For the smallest concentration, the error is 24%. The agreement is not very satisfactory, in particular as far as the slope of the curve for a larger etch depth is concerned.

In order to overcome this difficulty we can add another degree of freedom to the model and consider a finite density of surface states. Now we have to determine a pair (Φ^*, D_s) for exposed GaAs, and a pair for exposed AlGaAs.

In table 2 we show the sensitivities of N_{2DEG} to the four unknown parameters. The procedure of extraction is similar to that previously described: when N_a and N_d are determined, we have to evaluate the pair (Φ^*, D_s). For exposed doped $Al_{0.2}Ga_{0.8}As$ these values are obtained by fitting the slope of the electron density curve for larger etch values. D_s affects mainly the position of the knee of the curve in figure 6, while Φ^* the slope. Note how it is now possible to fit the slope of the experimental curve (thick curve). For exposed GaAs, Φ^* and D_s are obtained by fitting the slope of the electron density curve for small spacer thickness as shown in figure 7 (thick curves indicate experimental results, thin curves theoretical results). In table 3 we summarize the extracted parameters.

Table 2. Sensitivity of N_{2DEG} to parameters of the two-parameter model, in the case of exposed GaAs (left column) and in the case of exposed AlGaAs (right column).

	60 nm spacer thickness	1 nm etch depth
$S^{N_a}_{N_{2DEG}}$	0.15	0.14
$S^{N_d}_{N_{2DEG}}$	2×10^{-5}	0.13
$S^{\Phi*}_{N_{2DEG}}$	4×10^{-4}	8×10^{-4}
$S^{D_s}_{N_{2DEG}}$	2×10^{-5}	9×10^{-5}

6. Concluding remarks

We have presented a procedure for extracting important parameters required to perform accurate simulations of devices realized on GaAs/AlGaAs heterostructures, such as surface state parameters, and doping concentrations in the heterostructure.

We have also shown that a good agreement between experiments and simulations is obtained if a simple model based on two parameters is used to describe surface states, and that the improvement is significant with respect to the assumption of Fermi level pinning. Fermi level pinning is based on the assumption that the density of the surface states per unit energy is so large that an arbitrary charge can be induced on the surface with an infinitesimal variation of the Fermi level. As a second-order approximation, we assume that the variation of the Fermi level is finite but very small, so that only the density of surface states in the vicinity of the energy at which the Fermi level is quasi-pinned matters (our parameter D_s). A complete approach would require the complete knowledge of the density of surface states per unit energy. However, since surface states also depend on the fabrication process, such information can be hardly obtained from *ab initio* methods.

We believe that the two-parameter model used here represents a reasonable trade-off between, on the one hand, the need to provide an accurate description of surface states, and, on the other hand, the need to use a simple model, given the lack of information on surface states. While it is difficult to measure the predictive capabilities of such a model, because the characteristics of surface states depend on the fabrication process, the parameters extracted from the sample described in this paper have been used in the three-dimensional simulation of quantum point contacts defined by split gates on an AlGaAs/GaAs heterostructure, providing very good agreement with the experimental G–V curves of the QPCs [13]. The heterostructure on which the QPCs were defined was grown in the same laboratory and with the same process conditions as the test heterostructures considered in this paper. For this reason we have assumed the same surface state parameters.

Table 3. Summary of parameters providing the best fit for the GaAs/AlGaAs heterostructures in the case of the two-parameter model.

	Exposed GaAs	Exposed AlGaAs
N_a	3×10^{20} m^{-3}	3×10^{20} m^{-3}
N_d	5×10^{23} m^{-3}	5×10^{23} m^{-3}
D_s	5×10^{16} eV^{-1} m^{-2}	6×10^{16} eV^{-1} m^{-2}
$\Phi*$	4.85 eV	4.15 eV

Acknowledgment

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