Bistability and hysteresis in self-organised quantum dot structures

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Abstract. The hysteresis within the electron concentration versus gate voltage characteristic of a GaAs/*n*-AlGaAs field effect transistor with InAs quantum dots [G. Yusa, H. Sakaki, Appl. Phys. Lett., **70**, 345 (1997)] is investigated by a numerical approach. The calculations are based on the Poisson equation in combination with a drift-diffusion model including the electron capture and emission processes. Our simulations show that the hysteresis is of dynamical nature and that the Auger process is the suitable capture and escape mechanism to explain the experimental results.

1. Introduction

Field effect transistors (FET) with embedded InAs quantum dots (QD) [1] near a two dimensional electron channel show a distinct hysteresis in their electron concentration versus gate voltage characteristic [2] which makes them potentially applicable for a novel type of memory devices. The measurable shift in those characteristics with respect to up- and down-sweep remains from several seconds up to 100 hours [2, 3]. We investigate this bistable behaviour by a numerical approach and discuss different electron capture and escape mechanisms which suit with the experimental findings.

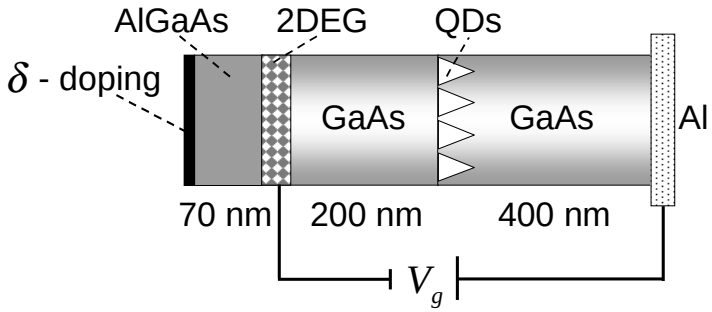

Figure 1. Sketch of the GaAs/*n*-AlGaAs field effect transistor with InAs QDs. The gate voltage V_g is applied between the two-dimensional electron gas and the Schottky contact (Al). The resulting conduction band edge is displayed in Fig. 3. The layers are (from left to right): $10^{12}/\mathrm{cm}^2$ δ-doping with Si; 70 *nm* $Al_{0.25}Ga_{0.75}As$ barrier; 200 *nm* GaAs; 1.75 monolayer InAs (dots); 400 *nm* GaAs; 100 *nm* Al as top gate.

Applying a voltage V_g to a device as shown in Fig. 1 fills the QDs with electrons. The charge captured within the QDs is detected by a change of the electron concentration within the two dimensional electron gas [2, 4]. In order to accomplish fast switching, the electrons

may be erased by light illumination [2, 3]. In this work we investigate the dark charging and discharging process.

The simulations of the experiment from Ref. [2] are performed as follows: We evaluate the conduction band edge with corresponding Quasi-Fermi level by the one-dimensional Poisson equation and continuity equation. The electron density in the QDs is determined by an electron capture and emission rate which also describes the dynamics in this system. A comparison of stationary and time-dependent calculation (see Fig. 2) displays the dynamical nature of the hysteresis during the up- and down-sweep. By assuming the Auger process with a rate equations coefficient C_{Auger} from Ref. [5] we find good agreement between theory and experiment. In contrast, for phonon assisted processes we have to use an extremely small capture rate to match the experimental behaviour. Therefore we can receive additional information regarding the electron capture in QDs [6, 7, 8] via modelling the hysteresis in this device.

2. Theory

The structure used in the experiment of Ref. [2] is shown in Fig. 1. The QDs exhibited a height $h = 5\ nm$ and a diameter 20 nm and the QD density was $(5-10)\times 10^{10} cm^{-2}$. For our calculations we estimate a ground state binding energy of $E_b = 250\ meV$ [9] and use the QD density $N_{QD} = 7.5\times 10^{10} cm^{-2}$.

The conduction band edge in Fig. 3 is determined by the intrinsic conduction band edge E_{c0} and the electric potential ϕ. We calculate the latter by solving self-consistently the one-dimensional Poisson equation (similar to Ref. [10])

$$
\begin{aligned}
&-\varepsilon_0 \frac{\partial}{\partial z}\left[\varepsilon_r(z)\frac{\partial}{\partial z}\phi(z)\right] = \rho(z) \\
&\text{with} \quad \rho(z) = e[N_D^+(z) - n(z) - n_{\mathrm{QD}}^{\mathrm{2d}}(t)\chi_{\mathrm{QD}}(z)]
\end{aligned}
\tag{1}
$$

where N_D^+ is the density of ionised donors resulting from the δ-doping, $n_{\mathrm{QD}}^{\mathrm{2D}}$ is the density per unit area of the electrons trapped within the QDs at position z_{QD}, n is the free electron density, ε_0 and ε_r are the absolute and relative permittivity. The characteristic function

$$
\chi_{\mathrm{QD}}(z) := \begin{cases} 1/h & (z \in \text{QD layer}) \\ 0 & (z \notin \text{QD layer}) \end{cases}
\tag{2}
$$

is used to reflect the finite extension of the QDs.

In order to calculate the Quasi-Fermi level E_F of the electrons we use the one-dimensional continuity equation

$$
-\frac{\partial}{\partial z}\left[\mu n(z)\frac{\partial}{\partial z}E_F(z)\right] = e f[n(z_{\mathrm{QD}}), n_{\mathrm{QD}}^{\mathrm{2D}}(t)]\chi_{\mathrm{QD}}(z)
\tag{3}
$$

with the electron capture rate f which determines the electron density in the QD layer (in units $\mathrm{sec}^{-1}\mathrm{cm}^{-2}$)

$$
\frac{\partial}{\partial t} n_{\mathrm{QD}}^{\mathrm{2D}}(t) = f[n(z_{\mathrm{QD}}), n_{\mathrm{QD}}^{\mathrm{2D}}(t)].
\tag{4}
$$

Here, $e > 0$ is the elementary charge and $\mu = 2\times 10^5\ \mathrm{cm}^2/\mathrm{Vs}$ is the electron mobility (at 77 K). This drift-diffusion approach is justified if the dielectric relaxation time is short compared to the dynamical time scales.

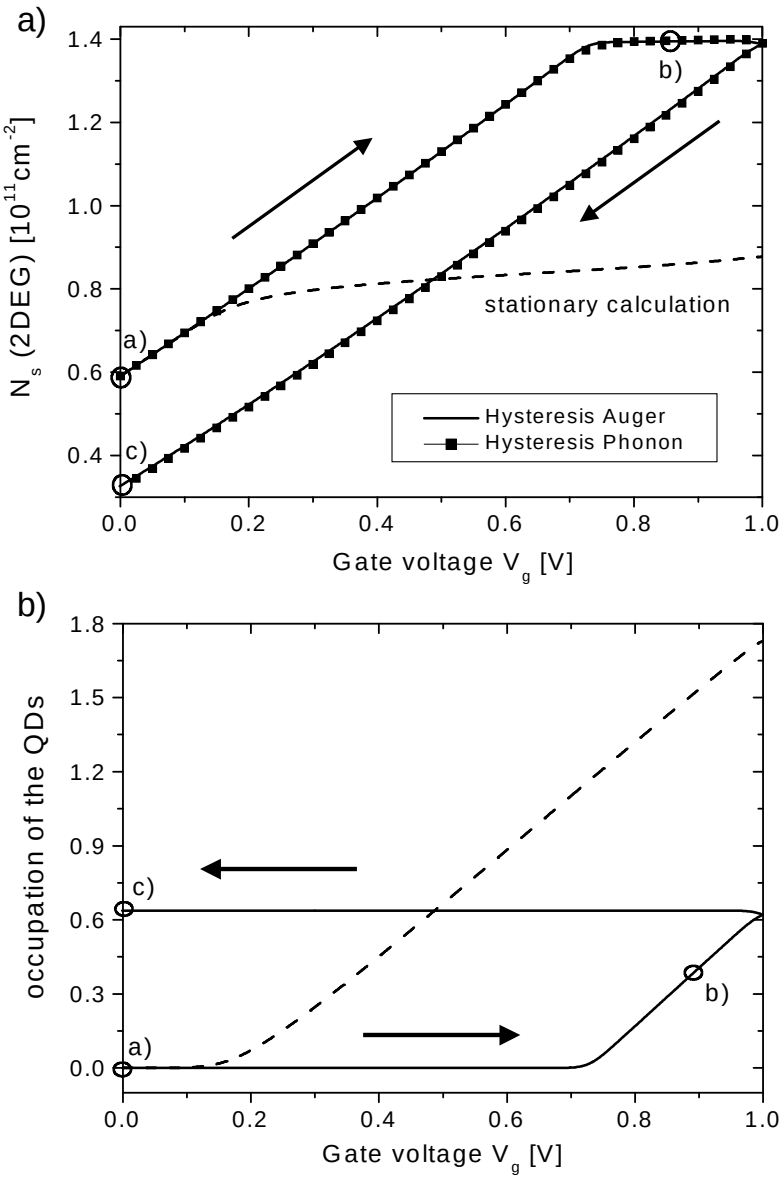

Figure 2. (a) Hysteresis in the channel electron density N_s versus gate voltage V_g characteristic. A sweep duration of 1 hour is supposed. For the Auger hysteresis we use $C_{Auger} = 2 \times 10^{-12} cm^4/s$ [5] and σ_{Phonon} is set to zero while for the phonon hysteresis $\sigma_{Phonon} = 2 \times 10^{-8} cm^2/s$ (fit) and $C_{Auger} = 0$. (b) the occupation of the QDs corresponding to the characteristic in (a). Three points are indicated within the plots – the corresponding conduction band edges can be seen in Fig. 3.

The standard expression for the free electron density is used [11]

$$n(z) = N_c(z) F_{1/2}\left(\frac{E_F(z) - E_{c0}(z) + e\phi(z)}{k_B T}\right)$$
$$\text{with} \quad N_c = 2\left(\frac{m_e k_B T}{2\pi\hbar^3}\right)^{3/2} \tag{5}$$

and the Fermi integral $F_{1/2}$. Here m_e is the effective mass, T the lattice temperature and k_B Boltzmann's constant.

The electron capture rate f is assumed to be a combination of Auger processes and single electron processes (like multi-phonon capture and emission) in the following way:

$$f[n, n_{\mathrm{QD}}^{2\mathrm{D}}] = (C_{Auger} n^{2\mathrm{D}} + \sigma_{Phonon})(n^{2\mathrm{D}} p_{\mathrm{QD}}^{2\mathrm{D}} - n_1^{2\mathrm{D}} n_{\mathrm{QD}}^{2\mathrm{D}}) \tag{6}$$

Here C_{Auger} and σ_{Phonon} are the rate coefficients for the Auger and multi-phonon process, respectively (see also Ref. [7]). $p_{\mathrm{QD}}^{2\mathrm{D}} = 2N_{\mathrm{QD}} - n_{\mathrm{QD}}^{2\mathrm{D}}$ is the density of unoccupied QD states for twofold degeneracy, $n^{2\mathrm{D}} = n(z_{QD})$ is the effective free electron density at the QDs per unit area (which may be related to a wetting layer density of the same order of magnitude), and the constant $n_1^{2\mathrm{D}} = N_c h \exp(-E_b/k_B T)$ results from the principle of detailed balance for equilibrium distributions in the nondegenerate case [12]. Quantisation effects in the two dimensional electron gas are neglected for simplicity. All calculations are performed at 77 K.

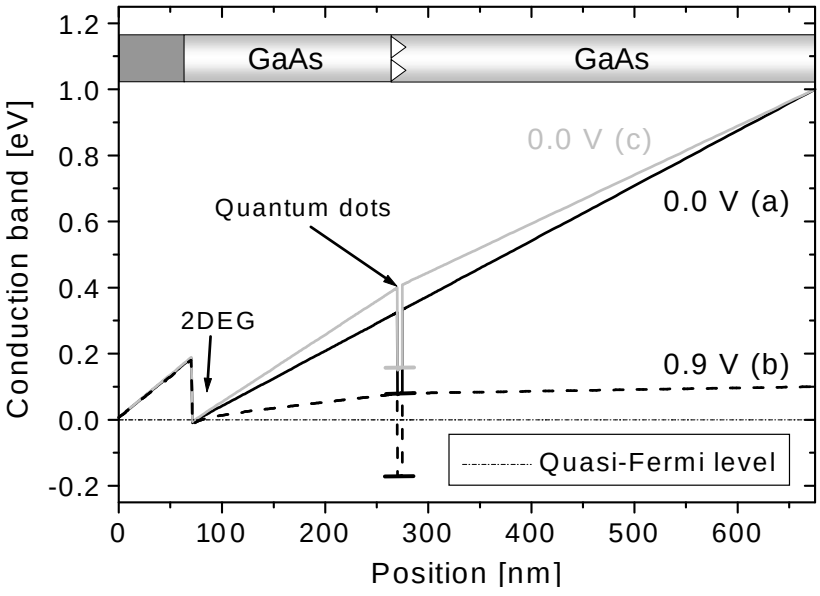

Figure 3. Calculated conduction band edges of the FET displayed in Fig. 1 for different gate voltages V_g. See Fig. 2 for the corresponding points within the hysteresis – indicated with (a), (b) and (c).

3. Results

At first we simulate the N_s-V_g-characteristic considering only the Auger process with $C_{Auger} = 2 \times 10^{-12} cm^4/s$ (calculated in Ref. [5]) and $\sigma_{Phonon} = 0$. The result is plotted in Fig. 2

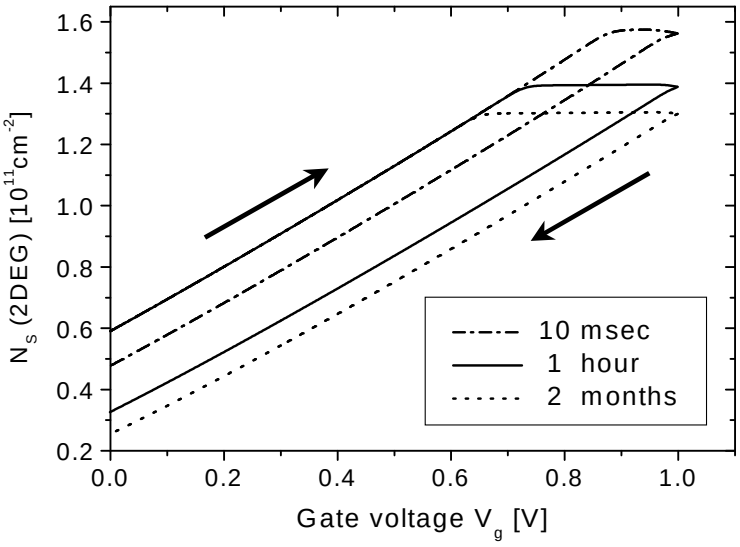

Figure 4. Hysteresis within the N_s-V_g-characteristic calculated with different sweep durations and an Auger coefficient of $C_{Auger} = 2 \times 10^{-12} m^4/s$ [5].

(a) – a simulated bias sweep from 0 V to 1 V and back (see the arrows in the plot) with a total duration of 1 hour shows a hysteresis as in Ref. [2]. In Fig. 2 (b) one can see that during the up-sweep starting at a gate voltage of ≈ 0.75 V the QDs are filled with electrons and that the electrons stay in the QDs during the down-sweep. Our results are in excellent agreement with the experimental data, see the broken line of Fig. 1 in Ref. [2]. In order to display the dynamical nature of the hysteresis we also calculated the stationary situation with $f[n, n_{\mathrm{QD}}^{\mathrm{2D}}] = 0$ – see the broken line in Fig. 2 (a). The clear difference between time-dependent and stationary calculation shows that both during up- and down-sweep nonequilibrium distributions persist. The capture and emission kinetics are not fast enough to establish thermodynamic equilibrium.

In combination with the calculated conduction band edges (see Fig. 3) we can analyse the origin of the hysteresis in detail. At the starting point (a) with zero voltage the QDs are empty, the QD energy level is far above the Quasi-Fermi level. Applying a gate voltage during the up-sweep moves the QD energy level below the Quasi-Fermi level – point (b). There the QDs are filled with electrons. During the down-sweep the electrons stay trapped within the QDs as the surrounding barriers are so high that the electrons can not be excited at low temperatures (see also Ref. [13]). The charge captured in the QDs is manifested in the difference of the conduction band edges between the starting point (a) and the end point (c) – see Fig. 3. In agreement with the experiment, the hysteresis disappears (stationary and time-dependent calculations deliver identical results) when a temperature of 300 K is used.

In order to display the robust behaviour of the N_s-V_g-characteristic against changing the time-scales involved we performed our simulations for different sweep durations. Fig. 4 shows our findings. One can see that the hysteresis slightly changes even if the sweep duration is changed by several orders of magnitude. This is even more interesting as for memory devices it is necessary to store charge at least for hours. With a more elaborate device structure as in Ref. [2] one was able to show that charge can be stored 100 hours at room temperature [3].

The capture kinetics from Eq. 6 dominates the dynamical behaviour. Now we want to

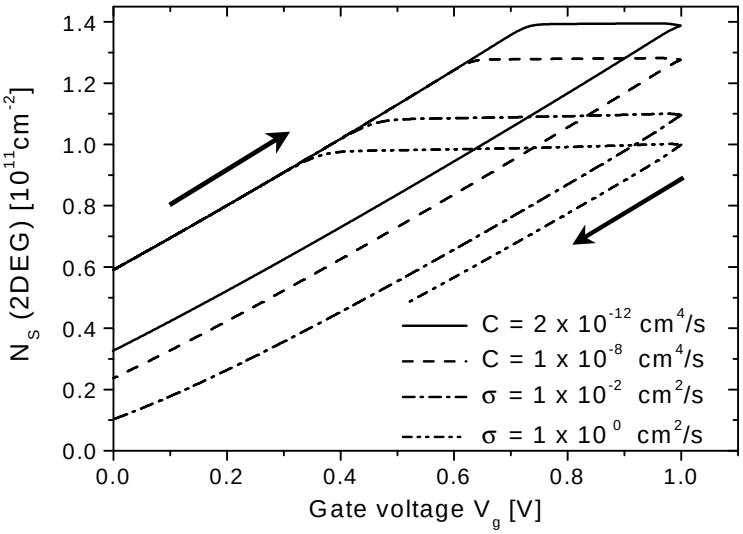

Figure 5. Calculated hysteresis in the N_s-V_g-characteristic for the Auger process and for the phonon processes only. Different coefficients for the rate equation and a sweep duration of 1 hour are used.

study the influence of different coefficients for Auger processes C_{Auger} and single electron processes σ_{Phonon}. As discussed before, the value of $C_{Auger} = 2 \times 10^{-12} cm^4/s$ [5] and $\sigma_{Phonon} = 0$ gives good agreement with the experimental findings. In Fig. 5 this characteristic (solid line) is given together with a calculation for $C_{Auger} = 10^{-8} cm^4/s$ [7] and $\sigma_{Phonon} = 0$ (dashed line). The latter result differs slightly and agrees less with the experimental data. Applying the single-electron capture coefficient $\sigma_{Phonon} = 1\ cm^2/s$ (from Ref. [7]) the result deviates strongly, see the dash-dotted line in Fig. 5 (here we used $C_{Auger} = 0$, the inclusion of $C_{Auger} = 10^{-8} cm^4/s$ hardly changes the result). While values of $\sigma_{Phonon} = 1\ cm^2/s$ or $10^{-2}\ cm^2/s$ (dash double-dot line in Fig. 5) strongly disagree with the experimental findings (the onset of the plateau occurs at far too low biases), extremely small capture rates $\sigma_{Phonon} = 2 \times 10^{-8} cm^2/s$ – see Fig. 2– yield good agreement.

Experimentally, one observes relatively fast capture rates at high electron densities, which are compatible with values of $\sigma_{Phonon} \sim 1\ cm^2/s$, see, e.g., Refs. [6, 7, 8]. Thus, single-electron capture processes are not able to explain both the fast capture at high electron densities and the rather long relaxation times observed in the FET device discussed here. In contrast, the Auger process depends quadratically on those densities, which goes well with both types of experimental observations. This demonstrates the relevance of the Auger process for the capture process in quantum dot structures.

4. Conclusion

In this work we presented a numerical simulation of a FET with InAs QDs. Our calculations show that the hysteresis observed in this quantum dot structure is of dynamical nature. The rather long time scales involved result from the quadratic dependence of the Auger process on the free electron density at the QDs which is quite low for small biases. Additionally, we could

analyse the dynamics leading to a hysteresis in the N_s-V_g-characteristic. A comparison of the Auger process with a possible phonon process showed that the Auger process with a capture coefficient of the order of $C_{Auger} \sim 10^{-8} - 10^{-12} cm^4/s$ goes well with the experimental findings – slow dynamics with low carrier densities and fast dynamics for high carrier densities. In contrast, single electron processes, such as (multiple) phonon assisted processes cannot explain both features with a single coefficient.

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