

Monte Carlo simulation of surface charge effects in T-branch nanojunctions

T. González¹, I. Iñiguez-de-la-Torre¹, D. Pardo¹, J. Mateos¹, S. Bollaert², Y. Roelens², and A. Cappy²

¹ Departamento de Física Aplicada, Universidad de Salamanca, Plaza de la Merced s/n 37008 Salamanca, Spain

² Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), Villeneuve D'Ascq, France

Received 5 July 2007, revised 8 August 2007, accepted 25 August 2007

Published online 11 October 2007

PACS 02.70.Uu, 73.20.-r, 85.35.-p

* Corresponding author: e-mail tomasg@usal.es, Phone: +34 923294436, Fax: +34 923294584

We analyze the influence of the surface charge on the operation of ballistic T-branch junctions based on InAlAs/InGaAs layers by means of a semi-classical 2-D Monte Carlo simulator. A new self-consistent model in which the local value of the surface charge is dynamically adjusted depending on the surrounding carrier density is used in the calculations. The

rectifying behaviour exhibited by these devices (down-bending shape of the output voltage V_C as a function of the applied voltage $V_R = -V_L = V$) is found to be much influenced by the surface charge. A satisfactory agreement is achieved between simulated results and experimental measurements.

© 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction The design and fabrication of new nanometer-sized electronic devices is a subject of growing activity in recent years [1–3]. As the smallest features of a device approach the nanoscale, the electronic properties of the constituent materials are increasingly affected by the surrounding surfaces and interfaces. In particular, in some nanodevices the sidewall surface charge, by depleting part of the conducting channel, plays a key role [4]. To analyze the physics of these devices by means of Monte Carlo (MC) simulations, surface states are typically modelled through a constant (neither depending on the position nor on the applied potential) negative surface charge density σ placed at the semiconductor-air interfaces [5]. This approach has been found to provide incorrect results when channels are very thin. Recently we proposed an improved model, based on the depletion induced by traps, in which the local value of σ is updated self-consistently with the carrier dynamics near the interface during the simulation [6]. In this work we apply such a model to investigate the influence of surface charges on the values of the output voltage V_C measured at the bottom of the (open circuited) vertical branch of T-shape three-terminal ballistic junctions (TBJs) [7] when several parameters of their geometry are modified; in particular, the width of the vertical branch W_{VER} , and the length L^{HOR} and width W^{HOR} of the horizontal branches (see Fig. 1).

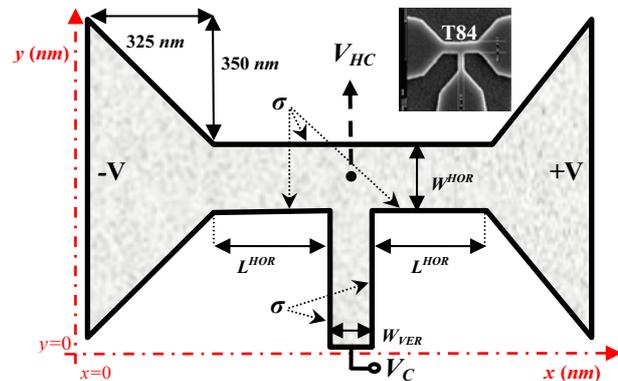


Figure 1 Schematic representation of the simulated T-branch junctions. The inset shows a SEM image of a TBJ with an 84 nm-wide central branch.

2 Physical model

2.1 Monte Carlo model We make use of a semi-classical ensemble MC simulator self-consistently coupled with a 2-D Poisson solver, where some assumptions, described in [5], are made to deal with the 3-D topology of real devices. To account for the fixed positive charges of the whole layer structure, a net background doping

$N_{Db}=10^{17} \text{ cm}^{-3}$ is considered when solving Poisson equation. A negative surface charge density σ , associated with the surface states, is assigned to the semiconductor-air interfaces (Fig. 1). The non-simulated dimension Z is estimated as $Z=n_s/N_{Db}=2\times 10^{-5} \text{ cm}$, with $n_s=2\times 10^{12} \text{ cm}^{-2}$, typical value of sheet electron density in the fabricated InAlAs/InGaAs channels. The output voltage V_C (Fig. 1) is calculated by averaging the electric potential (and subtracting the equilibrium value) at the bottom of the (open circuited) central branch when the horizontal branches are biased in push-pull fashion ($V_R=-V_L=V$).

2.2 Surface charge models An initial possibility to include the influence of surface charge in MC simulations is to consider a constant-charge model (CCM) in which σ is fixed to the experimentally-extracted equilibrium value ($\sigma/q=0.4 \pm 0.1\times 10^{12} \text{ cm}^{-2}$ for $\text{In}_{0.7}\text{Ga}_{0.3}\text{As}$ channels [8]), and kept constant independently of the topology of the structure, position along the interface, bias and time. While being adequate for thick branches, this model provides incorrect results for narrow channels (thinner than the theoretical depletion induced by the surface charge). To solve these problems we have recently proposed a self-consistent charge model (SCCM) able to reproduce more closely surface charge effects. The new model is based on the update of the local surface charge values according to the carrier density present in the nearby region [6]. First, the carrier concentration next to the boundary (N_{front}) is evaluated. Then, it is checked if N_{front} has a value in the range $[N_{low}, N_{high}]$, which represent the limits to which we try to adapt the electron concentration next to the interface. If the concentration (N_{front}) is higher than the upper limit (N_{high}), we increase the surface charge in a given amount $\Delta\sigma$. On the other hand if N_{front} is smaller than the lower limit (N_{low}), the surface charge is decreased in the same density $\Delta\sigma$. An optimization of the values of the parameters to improve the efficiency of the algorithm and the agreement with experimental results has been made. The selected values are $N_{low}=N_{Db}/100$, $N_{high}=N_{Db}/50$ and $\Delta\sigma=10^{-10} \text{ cm}^{-2}$. Every $N_i=500$ iterations the value of N_{front} is recalculated and the surface charge update algorithm is carried out. Neither the value of N_i nor that of $\Delta\sigma$ has been found to influence significantly the final results.

3 Fabricated and simulated devices The fabrication process and experimental characterization have been carried out at the IEMN, France. The InAlAs/In_{0.7}Ga_{0.3}As layer structure was grown by molecular beam epitaxy and the geometry of the TBJs was defined by a high resolution negative e-beam resist, Hydrogen Silses Quioxane, exposed by a LEICA EBPG5000+ machine, and CH₄/H₂/Ar reactive ion etching [8]. Several TBJs with different widths of the vertical branch W_{VER} (from 66 to 108 nm) were fabricated. A scanning electron microscope (SEM) image of the TBJ with 84 nm wide vertical branch is shown in Fig. 1. Contact resistances of 650 Ω are considered in the simulations to account for the potential drop in the non simulated

portion of the accesses (of the order of 300 nm) [9]. In all the TBJs, the length and width of the horizontal branches are $L^{HOR}=250 \text{ nm}$ and $W^{HOR}=170 \text{ nm}$, respectively. Simulations and experimental measurements were performed at room temperature (300 K).

4 Results and discussion Typically, the vertical branch of TBJs is considered to act as a passive element [7], so that V_C is expected to be independent of its width W_{VER} . However, the experimental measurements of V_C (performed with a high-impedance voltmeter) shown in Fig. 2(a), corresponding to TBJs with narrow vertical branch, exhibit a different behaviour. The narrower the width of the branch, the higher (more negative) the measured value of V_C . As concerns the current flowing through the horizontal branches I , shown in the inset of Fig. 2(a), as expected, it is independent of W_{VER} , since these branches are practically identical for the different TBJs. When trying to reproduce these measurements with MC simulations using the CCM, the results are totally inconsistent with experiments due to the fact that for narrow branches the depletion region that surface charges should

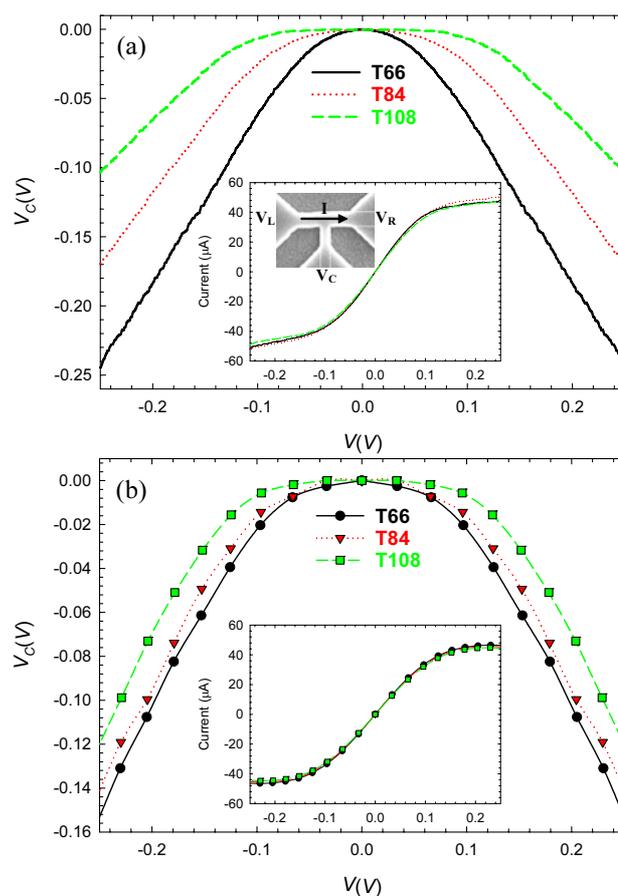


Figure 2 (a) Experimental and (b) MC values of the bottom potential V_C and current (insets) in the TBJ junctions with $W_{VER} = 66, 84$ and 108 nm (denoted as T66, T84 and T108, respectively) as a function of the push-pull bias V .

induce is wider than the real width of the branches, so that charge neutrality is not ensured and unphysical negative potentials are obtained. In contrast, the calculations of V_C performed with the SCCM, reported in Fig. 2(b), are consistent with the experimental results, showing the same trend (higher negative values for lower W_{VER} , with quadratic shape at low bias) and a rather good quantitative agreement. In particular, the agreement is excellent for the TBJ with the wider vertical branch (T108). In the case of the current [insets of Figs. 2(a) and (b)], measurements and simulations match almost perfectly for the whole set of junctions, both qualitatively and quantitatively.

Results in Fig. 2 indicate that in the TBJs under analysis the vertical branch is not just a voltage probe which reflects the variations of the voltage at the centre of the horizontal branch V_{HC} . As observed in Fig. 3, which compares V_C and V_{HC} in T66 and T108, V_C is not a faithful reflection of V_{HC} . This is due to the presence of surface charges at the lateral walls of the vertical branch. As expected, the values of V_{HC} hardly depend on the width of the central branch, and even on the presence or absence of this branch (since the values coincide with those calculated in a channel without vertical branch, dashed line). Therefore, the dependence of V_C on the width of the vertical branch W_{VER} is a vertical effect associated with the changes (among the different TBJs) in the profiles of the electrostatic potential along the vertical branch induced by the surface charges [6]. In the inset, the improved parabolic behaviour obtained with the SCCM as compared with the CCM is observed. The SCCM leads to a significant increase of the negative values of V_{HC} for a given bias as a consequence of an enhanced surface charge asymmetry in the horizontal branch [6].

Apart from the fitting of the measurements performed in the TBJs with different W_{VER} fabricated at the IEMN, our

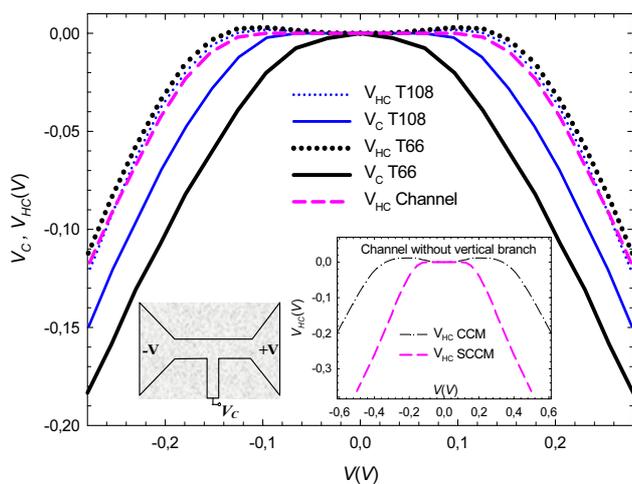


Figure 3 V_{HC} and V_C as a function of the applied voltage for the TBJs with $W_{VER} = 66$ and 108 nm. V_{HC} for a channel without vertical branch is also plotted for comparison. The inset shows V_{HC} calculated in the channel without vertical branch with the CCM ($\sigma/q = 0.4 \times 10^{12} \text{ cm}^{-2}$) and SCCM models of surface charge.

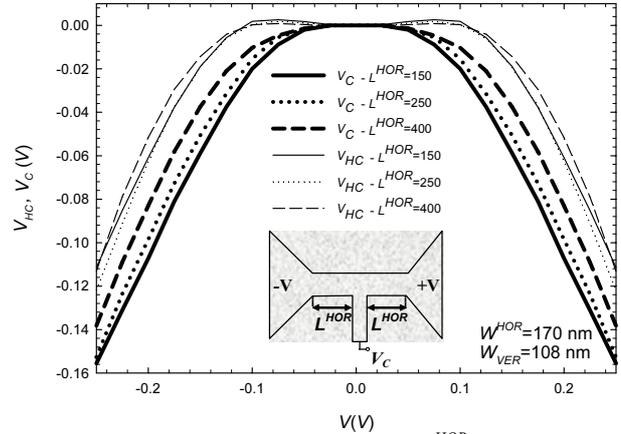


Figure 4 $V_{HC}-V$ and V_C-V for TBJs with $L^{HOR} = 150, 250,$ and 400 nm.

surface charge model can also be applied to interpret the experimental behaviour found in similar TBJ structures, recently reported in the literature [10], where the length L^{HOR} and the width W^{HOR} of the horizontal branches are modified. We will take as a basis the structure with $W_{VER} = 108$ nm previously analyzed, in which the values of L^{HOR} and W^{HOR} will be changed. As will be shown in the following, the qualitative behaviour of our MC simulations coincides with that found experimentally. A quantitative agreement is far from the objectives of this work, since for comparison we will simulate structures similar to those fabricated at the IEMN are not the TBJs measured in [10]. Figure 4 shows the results obtained by modifying the length of the horizontal branches L^{HOR} , for $W_{VER} = 108$ nm. The values of V_{HC} are very similar for all the structures. This is due to the analogous horizontal concentration profiles found for the different lengths, so that the potential drop from the contacts to the centre of the junction is practically the same. As in the previous TBJs, it is the presence of the vertical branch and the associated surface charges which induce different values of V_C in each of the structures. Like in the case of the experimental results reported in [10], we find that the down-bending behaviour of V_C is stronger for shorter junctions. This result is expected because of the more ballistic character of transport in shorter structures, but our results indicate that surface charges and the presence of the vertical branch also play a role.

Finally, Fig. 5 shows the values of V_{HC} and V_C in TBJs where the width of the horizontal branch W^{HOR} is modified, for $L^{HOR} = 250$ nm and $W_{VER} = 108$ nm. As observed, the values of V_C are higher (more negative) as the width is decreased, in accordance with the trend found in experiments [10]. Remarkably, and in contrast with the behaviour found when modifying W_{VER} and L^{HOR} , in this case the values of the potential at the centre of the junction V_{HC} exhibit a strong dependence on W^{HOR} . In these structures, despite the length is the same, the profile of carrier concentration along the horizontal branch depends strongly on its width due to the depletion induced by the surface charges, as observed in Fig. 6. As expected, carrier concentration at the

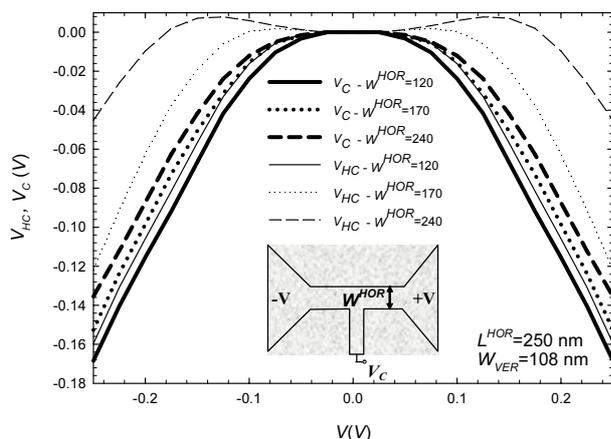


Figure 5 $V_{HC}-V$ and V_C-V for TBJs with $W^{HOR} = 120, 170,$ and 240 nm.

centre of the horizontal branch is lower for smaller W^{HOR} due to the more pronounced depletion. For this reason, the horizontal profile of electric potential changes significantly with W^{HOR} , and consequently the values of V_{HC} are different in each TBJ. Such differences are smoothed along the vertical branch by the influence of surface charges, but are still noticeable at its bottom, in the values taken by V_C .

In Fig. 6, a remarkable asymmetry is observed in the electron carrier density profile, originated by the combined effects of quasiballistic transport and surface charge asymmetry (enhanced by the SSCM, as mentioned previously). Due to the lower electron concentration, most of the applied voltage drops in the anode region, leading to the high negative values of V_{HC} (and V_C).

5 Conclusion The rectifying behaviour of TBJs with different topologies has been analyzed by means of a 2D ensemble MC simulator which implements a new self-consistent surface charge model. The characteristic quadratic output voltage of TBJs, $V_C = -\alpha V^2$, is found to be

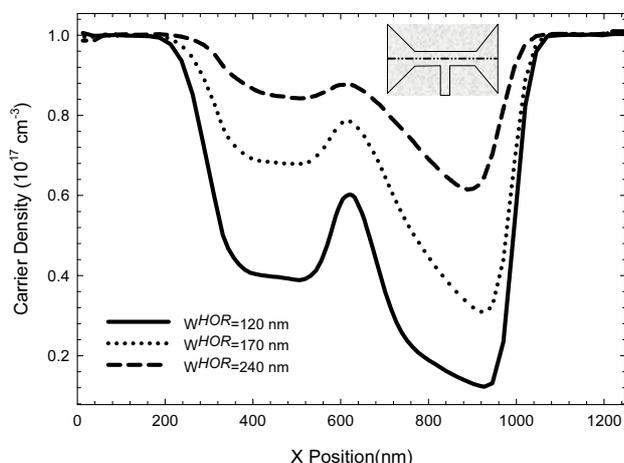


Figure 6 Electron concentration along the centre of the horizontal branch for different W^{HOR} for a bias $V = 0.25$ V.

much influenced by the size of the different branches. The self-consistent surface-charge model provides a good qualitative description of the operation of TBJs fabricated with different width of the vertical branch, yielding higher negative values for V_C as W_{VER} is decreased. The current flowing through the horizontal branches has been quantitatively reproduced in a totally satisfactory way. As long as the vertical branch is narrow enough, the bias dependence of the surface charge and electron concentration inside it originates that the variations of the potential at the centre of the TBJs V_{HC} are not transmitted in the same way to the bottom of the vertical branch when its width is modified. The influence of the length and width of the horizontal branches has also been analyzed and found to agree qualitatively with experimental findings in the literature.

Acknowledgements This work has been partially supported by the Dirección General de Investigación (MEC, Spain) and FEDER through the project TEC2004-05231 and by the Consejería de Educación of the Junta de Castilla y León (Spain) through the project SA044A05.

References

- [1] L. Worschech, D. Hartmann, S. Reitzenstein, and A. Forchel, *J. Phys.: Condens. Matter* **17**, R775 (2005).
- [2] A. M. Song, in: *Encyclopedia of Nanoscience and Nanotechnology*, edited by H. S. Nalwa (American Scientific Publishers, Stevenson Ranch, 2004), pp. 371-389.
- [3] L. Bednarz, Rashmi, P. Simon, I. Huynen, T. González, and J. Mateos, *IEEE Trans. Nanotech.* **5**, 750 (2006).
- [4] A. M. Song, M. Missous, P. Omling, I. Maximov, W. Seifert, and L. Samuelson, *Appl. Phys. Lett.* **86**, 042106 (2005).
- [5] J. Mateos, B. G. Vasallo, D. Pardo, T. González, J. S. Galloo, Y. Roelens, S. Bollaert, and A. Cappy, *Nanotechnology* **14**, 117 (2003).
- [6] I. Iñiguez-de-la-Torre, J. Mateos, T. González, D. Pardo, J. S. Galloo, S. Bollaert, Y. Roelens, and A. Cappy, *Semicond. Sci. Technol.* **22**, 663 (2007).
- [7] I. Shorubalko, H. Q. Xu, I. Maximov, P. Omling, L. Samuelson, and W. Seifert, *Appl. Phys. Lett.* **79**, 1384 (2001).
- [8] J. S. Galloo, E. Pichonat, Y. Roelens, S. Bollaert, X. Wallart, A. Cappy, J. Mateos, and T. González, in: *Proc. 2004 International Conference on Indium Phosphide and Related Materials*, IEEE Catalog 04CH37589, pp. 378-381 (2004).
- [9] J. Mateos, B. G. Vasallo, D. Pardo, T. González, E. Pichonat, J. S. Galloo, S. Bollaert, Y. Roelens, and A. Cappy, *IEEE Electron Device Lett.* **25**, 235 (2004).
- [10] D. Wallin, I. Shorubalko, H. Q. Xu, and A. Cappy, *Appl. Phys. Lett.* **89**, 092124 (2006).