Study of the high-frequency performance of III-As nanojunctions using a three-dimensional ensemble Monte Carlo model

To cite this article: Toufik Sadi and Jean-Luc Thobel 2009 J. Phys.: Conf. Ser. 193 012017

View the article online for updates and enhancements.
Study of the high-frequency performance of III-As nanojunctions using a three-dimensional ensemble Monte Carlo model

Toufik Sadi and Jean-Luc Thobel

Institut d’Electronique, de Microélectronique et de Nanotechnologie (IEMN), UMR-CNRS 8520, Université Lille 1, 59652 Villeneuve d’Ascq Cédex, France
E-mail: Toufik.Sadi@IEMN.Univ-Lille1.fr

Abstract. We apply a well-calibrated three-dimensional Monte Carlo simulator using finite-element meshing to study the intrinsic high-frequency (HF) behaviour of three-terminal nanojunctions based on InGaAs/InAlAs heterostructures. To obtain a reliable prediction of device performance, we use a realistic model for surface charge effects at high-frequency conditions. In this work, we perform an analysis of the dynamics of electron transport in the devices and present a prediction of their intrinsic HF performance. The results demonstrate the suitability of these nanostructures for application in the terahertz regime, and illustrate the influence of surface charge effects in this frequency range.

1. Introduction
It is widely accepted that future improvement in device performance should not be expected from size reduction but rather from profound change in geometry. In this context, the development of reliable three-dimensional (3D) simulation tools are essential to help designers to determine the best structures, and provide insight into their physical behaviour which is still not completely understood especially at high-frequencies. The use of nanojunctions has been suggested as one possible solution to the scaling problem. Such structures have attracted substantial interest in recent years, due to their non-linear properties [1]. We report results from the study of the intrinsic high-frequency (HF) behaviour of T-branch junctions (TBJs) based on InGaAs/InAlAs heterostructures, using a 3D Monte Carlo simulator. TBJs incorporating InGaAs channels are promising for terahertz applications due to the high 2DEG mobility in these structures. These nanodevices function as voltage rectifiers, under a push-pull biasing scheme, due to quasi-ballistic transport and surface charge effects in these devices. TBJs can also be used in logic circuits as Multiplexer/Demultiplexer (MUX/DEMUX) structures, as discussed below. The simulated TBJs are shown in Fig. 1. Details of the InGaAs/InAlAs heterostructure are given in [1].

2. Simulation Model, Results and Discussion
The simulator self-consistently couples 3D non-equilibrium electron dynamics with a solution of the 3D Poisson’s equation using the finite-element method [2]. As demonstrated in [1], the correct inclusion of the real device geometry in the 3D space is necessary for the accurate analysis of electron transport, which is important to understand the physics of these devices. The model
Figure 1. (left figure) TBJ structure simulated by applying a push-pull biasing scheme to study rectification, by observing the output potential $V_C$. (right figure) The TBJ structure with a gate contact used as a MUX/DEMUX structure. See [1] for more details about these structures.

minimises significantly the need for parameter fitting to match experimental results, and leads to more realistic macroscopic and microscopic characteristics. The simulator incorporates a realistic surface charge model designed specifically for HF simulations. This is necessary since surface charge effects play an important role in the performance of these devices characterised by a relatively high surface-to-volume ratio. The newly-developed charge model is partially based on the model used in our previous work for DC analysis [1], and allows the adjustment of surface charge density according to electron concentrations near the free surfaces. To reduce the computational cost, the applied potentials at terminals $T_1$ ($V_L$) and $T_2$ ($V_R$) are assumed to follow a squarewave form, with the same frequency $f$. In general, the biasing scheme chosen such that push-pull polarisation is maintained at every instant of the simulation. In the first half-period (case 1) $V_L$ is set to $-V_1$ and $V_R$ is set to $+V_1$, while in the second half-period (case 2) $V_L$ is set to $+V_2$ and $V_R$ is set to $-V_2$. The HF charge model is applied as follows. First, we perform DC simulations to determine the fixed charge distribution in each surface of the device, for both biasing cases (we use $\sigma_1$ to define the charge density at a given surface for case 1, and $\sigma_2$ to define the charge density for case 2). Since little is known about the fixed charge at the surfaces we suggest three models for considering surface effects at HF conditions. The first model (Model I) allows instantaneous change of $\sigma$ (from $\sigma_1$ to $\sigma_2$ or vice-versa) with the applied potential. The second model (Model II) allows a time-dependent change of $\sigma$: if a change in the applied potential occurs from case $m$ to case $n$ ($m = 1, 2$, $n = 1, 2$), $\sigma$ is given by

$$\sigma = \sigma_m + ([\sigma_n - \sigma_m])(1 - \exp\{-t/\tau\} + \exp\{-T/2)/\tau]/2).$$

(1)

t is the time elapsed since the last potential change, $\tau$ is the time constant and $T$ is the time period. The third model (Model III) sets the value of $\sigma$ to the average value ($\sigma_1 + \sigma_2)/2$. Clearly, Models I and III represent special (opposite) cases of Model II, corresponding to $\tau \sim 0$ and $\tau \sim \infty$, respectively. The simulations are run assuming room temperature (300 K).

For the analysis of the simple TBJ structure (without a gate contact) shown in Fig. 1, we generate results at 1THz. The biasing scheme is chosen such that push-pull polarisation ($V_L = -V$ and $V_R = V$) is satisfied in the first half-period. In the second half-period, both $V_L$ and $V_R$ are set to zero. In the case of Model II, $\tau$ is set to $T$ for the sake of illustration. Fig. 2 shows the variation of the average $V_C$ (representing the central potential at the bottom of the vertical branch) with bias for the three charge models, for 1THz as well as for the DC case. In Fig. 2, we also show the time dependence of $V_C$, at a high bias. The results demonstrate how the choice of the charge model influences considerably the predicted results. Model I gives a
strong time-dependence of $V_C$. In this case, the electron population does not settle to a steady state, leading to unrealistic average $V_C$ values. Model III gives a much less time-dependence of $V_C$. While both models represent extreme cases of the influence of surface charge, model III may be more suitable at high frequencies, since the surface charge is expected to respond relatively slowly to bias changes. At 1THz, this model is shown to give results that are similar in both half-periods, suggesting that surface charge effects may be an important factor in determining the HF behaviour of TBJs. Such possibility leads to an important conclusion: For an improved performance at high-frequencies, future designs should incorporate a reduced junction length to minimise the influence of surface charge effects, and enhance the role of ballistic transport on the switching behaviour of TBJs. In general, realistic results are expected to lie between these two extremes, by choosing, for example, a time constant value $\tau$ (see Fig. 2) from calibration with HF experimental data, which are not available at the moment.

For a deeper understanding of the physics governing device operation at high frequencies, we show in Fig. 3 the variation of the mean electron velocity and energy along the channel. The results are taken at the $z$ coordinate ($z_{HC}$) corresponding to the middle of the device (see Fig. 1). These results are shown for the first-half period ($V_L = -0.3$, $V_R = +0.3$). As discussed above, model I leads to unrealistic results. In this case, microscopic results show a significant reduction in the average velocity, which is verified to be due to an increase in electron transitions to the upper valleys. Analysis of the microscopic results obtained from models II and III show the expected asymmetry in velocity and energy. The average (and peak) velocities and energies are reduced at higher frequencies. The energy profiles, showing a constant increase in electron energy in the junction, are maintained at 1THz. These profiles, which are at the origin of the rectifying behaviour of TBJs, suggest that such devices maintain their non-linear behaviour at high frequencies, and therefore are suitable for terahertz applications.

TBJs can be used as MUX/DEMUXs for logic applications [3], by introducing a Schottky gate contact in the structure, as explained in [1]. We apply the simulator to demonstrate the device operation at high frequencies but also the influence of surface charge effects. Fig. 1 shows this structure and the biasing scheme used for this study. The applied gate potential $V_G$ is assumed to follow a squarewave form with a frequency of 1THz. The magnitudes are $+0.75V$ in the first half-period and $-0.75V$ in the second half-period. When $V_G$ is positive most of the current flows through terminal $T_2$ ($I_2$), and when $V_G$ is negative most of the current flows through terminal $T_3$ ($I_3$). This explains its characteristic as a MUX/DEMUX. Fig. 4 shows the variations of the current with time, when using models I and II ($\tau = T$). While
Figure 3. Variations of (left figure) the mean electron velocity in the x direction and (right figure) kinetic energy in the channel at $z = 0.21\mu m$ and $V = 0.3V$. The results are obtained from the three surface charge models, for a frequency of 1THz. DC results are also shown. The vertical line shows the centre of the device in the x direction.

Figure 4. Time-variations of (left figure) $I_2$ and (middle figure) $I_3$, for a 1THz frequency and surface charge model I. The figure on the right shows the variation of $I_2$, for surface charge model II, for the same frequency.

the MUX/DEMUX function is maintained at 1THz, surface charge models give considerably different average current values, demonstrating the importance of understanding surface charge effects for a complete understanding of the behaviour of nanojunctions at high-frequencies.

3. Conclusions
This work presents an analysis of the intrinsic high-frequency behaviour of III-As TBJs, using a 3D Monte Carlo simulator incorporating a finite-element Poisson solver. Results demonstrate how the behaviour of the devices as switches is sustained at the terahertz frequency range, and most importantly illustrate the role played by surface charge effects in this regime.

Acknowledgments
The authors would like to thank F. Desenne from the IEMN for valuable discussions.

References