

TCAD Simulation for Advanced Terahertz SiGeC HBTs

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Abstract. This paper deals with the physical modeling and accurate simulation of SiGeC Heterojunction Bipolar Transistors. An original methodology of TCAD simulation for advanced SiGeC HBT in BiCMOS technology is presented. This novel approach includes both process simulations for all the fabrication steps and electrical analyses, rigorously taking into account the process-dependent material properties.

The benefits of the carbon incorporation into the base have been demonstrated on the electrical behavior of HBTs but its impact is frequently ignored in the modeling. Present work uses state of the art of physical models (low-field mobility, saturation velocity, energy relaxation time, etc.). Hydrodynamic (HD) mixed-mode simulations were performed. The electrical results of the simulated device and critical figures of merit of HBTs (Gummel plot, Maximum oscillation frequency and unity-current gain transition frequency) are validated showing an excellent agreement with measurements.

The proposed methodology may be used to obtain more physical and realistic results, better understanding of charge transport, and facilitate HBT device development and optimization.

Keywords: Heterojunction Bipolar Transistor (HBT), TCAD, Silicon Germanium, SiGeC, Monte Carlo, Device simulation, Device Physics.

1. Introduction

Technology Computer Aided Design (TCAD) has become an important tool for the development and optimization of new semiconductor technologies. Accurate TCAD used dedicated models for the technology process including all process steps and dedicated models to simulate the electrical behaviour of the device.

Over the years, models have been enhanced jointly with the technological progress, using new materials, structures and reducing the overall device dimensions for higher operation speed. An accurate modelling of the device depends on two aspects: 1/ the ability to describe the real structure of the device with for instance doping and composition profiles up to the nano-scale, 2/ the physical model used to simulate the electrical behaviour of the device. For the first aspect, the structure can be completely drawn according to structural/dimensional characterisation of the real device, or the structure can be the results of the modelling of the fabrication processes as deposit/growing, etching, implantation, annealing. In the second case, TCAD can be used for prediction and for an optimization of the process flow. For the second aspect, the results could be very accurate if the charge transport mechanism at the microscopic level is included but suffering from computation limitation for the whole device. Then some approximations can be made such an averaging of the transport mechanisms, and by neglecting second order phenomena. Wrong results appear when modelling is used out its valid domain. Assumptions are done for modelling according to experimental results but it is difficult to deal with many parameters with many mixed physical mechanisms involved in DC and AC results.

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In TCAD simulation for SiGeC HBTs, the impact of carbon incorporated into the base is frequently ignored in the device simulation. Different studies have shown the interest to use carbon to reduce the boron diffusion in strained SiGe base layers [1]-[2]. This reduction is achieved by the under-saturation of Si self-interstitial caused by the out-diffusion of C [3]-[4]. A more doped and thinner base leads to improve device frequency performances. Unfortunately, the carbon has not only a beneficial impact on transistor behaviour. If the C content in silicon is above 2%, it can severely degrade transistor's performance [5]. Carbon atom placed in interstitial sites can create nano-crystalline SiC clusters, recombination centers and generate significant leakage currents [6]. Predictive hydrodynamic (HD) simulation of SiGeC HBT where base layers are biaxially strained on Si, requires taking into account the combined effects of the ternary alloy specific properties, and the biaxial stress induced by the lattice mismatch. In this paper, we carried out HD simulations with Monte Carlo (MC) based analytical models for SiGeC alloys [7]- [9] implemented in the simulator SDevice [10]. The simulated device is based on the mature technology BiCMOS9MW developed by STMicroelectronics [11]-[12], and fabrication process steps were updated in order to obtain a HBT of B3T Technology [13] featuring figures-of-merit f_T of 260 GHz and f_{MAX} of 350 GHz, which was elaborated in the frame of the Dotfive European project [14].

2. SiGeC Alloy Specific Models

Incorporation of Ge and C atoms in silicon modifies the lattice parameter, and therefore the electronic structure. SiGeC can be used with Si to build heterojunctions and gradual composition layers, with appropriated potential barrier and static electric field,. The transport properties of the carriers are modified at the material level which leads to a modification at the device level. A rigorous modeling of carriers transport must consider these changes to simulate their possible impact on the device behaviour [9]. In advanced tools as full band MC, the effects induced by the stress and composition of the material are inherently taken into account in the band structure and interaction models. Table I shows properties of silicon, germanium and carbon at room temperature.

Table 1 Properties of Si, Ge and C at Room Temperature.

Parameter	Si	Ge	C	Unit
E_g	1.12	0.66	5.47	eV
a	5.43	5.66	3.57	Å
ρ	2.33	5.32	3.52	g/cm ³
ϵ	11.90	16.20	5.70	-

The use of Full-Band MC method enables the simulation of carrier transport at high energies, up to 3 eV. Equipped with these numerical models, MC programs are able to simulate the electrical properties of materials subject to strong electric fields.

The MC based analytical model used in our HD simulations was developed for doped ternary $Si_{1-x-y}Ge_xC_y$ alloys, relaxed or biaxially strained on a silicon substrate. It describes homogeneous and stationary transport of both electrons and holes; the band structure description is made by a numerical Full-Band method. Modelled mechanisms include ionized impurity scattering, alloy scattering, carrier-phonon scattering and impact ionization. For material parameters extraction and the analytical models formulation, the SiGeC transport parameters include the Ge and C relative concentration, the type of active doping species, the crystal lattice temperature, and the external electric field and biaxial stress effects.

Charge carrier mobility was calculated based on low-field MC simulations; it includes physical dependencies upon Ge, C and doping concentrations. Band structures are modelled based on strain-dependent SiGe Tight-Binding [14].

3. Process Simulation

TCAD simulations are performed based on the full description of every processing steps of the B3T technology developed at STMicroelectronics [13]. Briefly, the device obtained from this technology is a double-polysilicon fully-self aligned (FSA) HBT, with a selective epitaxial growth (SEG) B-doped SiGeC base, an As-doped mono-emitter and a collector module formed by: an n+ buried layer, collector epitaxy and a selectively implanted collector (SIC). The B3T simulated HBT is derived from the BiCMOS9MW technology; it was released in DotFive European project [14] in order to obtain a HBT SiGeC device which reaches a maximum oscillation frequency (f_{MAX}) higher than 500 GHz. Each processing step of the process flow was carefully simulated with the aim of obtain accurate prediction of the active dopant distribution, of the stress distribution and of the final device geometry of the device.

3.1. 1D Process Simulation

A one-dimensional modelling of the process is performed in order to simulate accurately the vertical profile of dopants grown through the emitter window of the HBT. Base epitaxy is formed with a Ge graded profile, increasing from 20% at the emitter side up to 30% at the collector side of the base. The B and C incorporation during epitaxy are also simulated according to process flow. SEG is finished with a silicon cap layer, which will form the mono-emitter once As-doped poly-silicon deposition and diffusion is done.

Simulated device has a C content lower than 1%, this percentage blocks B diffusion and allows a higher doping level of B. A thin base is then obtained with the objective to improve the HBT electrical behaviour.

3.2. 2D Process Simulation

A 2D modelling of the NPN transistor is also performed to accurately simulate collector and sinker doping profiles formed by implantation-diffusion in silicon. The Boron diffusion out of the extrinsic poly-silicon base layer and through the poly-silicon interface into the intrinsic base layer is one of the major new modelling done here because of the impact of the whole base doping profile on f_{MAX} performances and on device lateral reduction capability.

The use of FSA-SEG architecture [14]-[15] gives many advantages over previous generations. A complete emitter-base-collector alignment is possible by performing SIC implantation through the emitter window. The intrinsic device is thus achieved with only one level of photolithography. There is not mismatching risks, base and collector contacts can be closer to the center of the device, which will reduce the base resistance and therefore, increases f_{MAX} .

Main regions of the 2D structure were set as tuneable parameters in the process simulation. It allows variations in L-shape emitter-base (EB) spacer length and thickness, in nitride spacer thickness, in base-collector (BC) oxide thickness and in external-to-internal base connection length. By varying these parameters we obtained a structure more similar to real HBT observed with TEM pictures and subsequently realistic results. It can be used also to simulate different technology splits, or evaluate the impact of the structure parameters on the device characteristics.

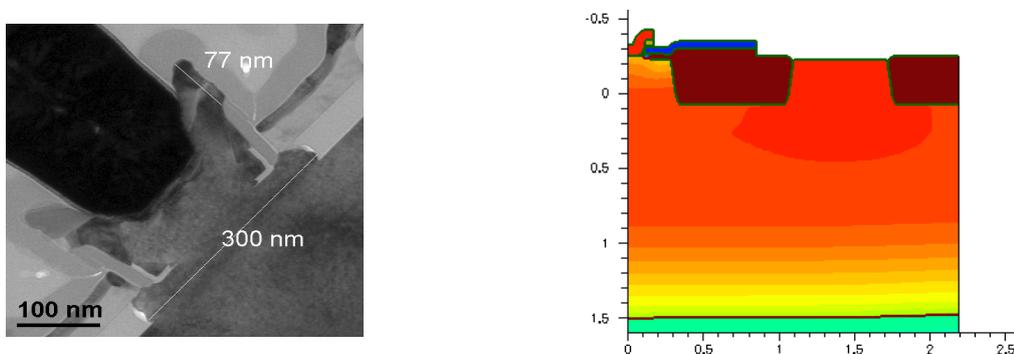


Fig. 2. a) TEM cross-section of the simulated device. FSA-SEG SiGeC HBT with emitter width (WE) of 130nm; b) TCAD Cross Section of a SiGe HBT elaborated under B3T technology process flow.

4. Electrical Simulation

Mixed-mode simulations for the HBT final structure were performed. The electrical results of simulated device are validated comparing simulation with the experimental measurements showing an excellent agreement. We compared the main figures of merit for HBTs: Gummel plot, Maximum oscillation frequency (f_{MAX}) and unity current gain transition frequency (f_T) which are the main figures of merit for HBTs.

4.1. Electrical Results

Fig. 3 shows the comparison of the electrical characteristics between the simulated structure and measurement. DC results are compared with a Gummel plot, and AC results are compared with f_{MAX} versus the collector current I_C , at $V_{CB} = 0$ V at 300 K. Simulation is with the SiGeC advanced models, and measurements are from a device with an effective emitter area of $0.13 \times 10 \mu m^2$.

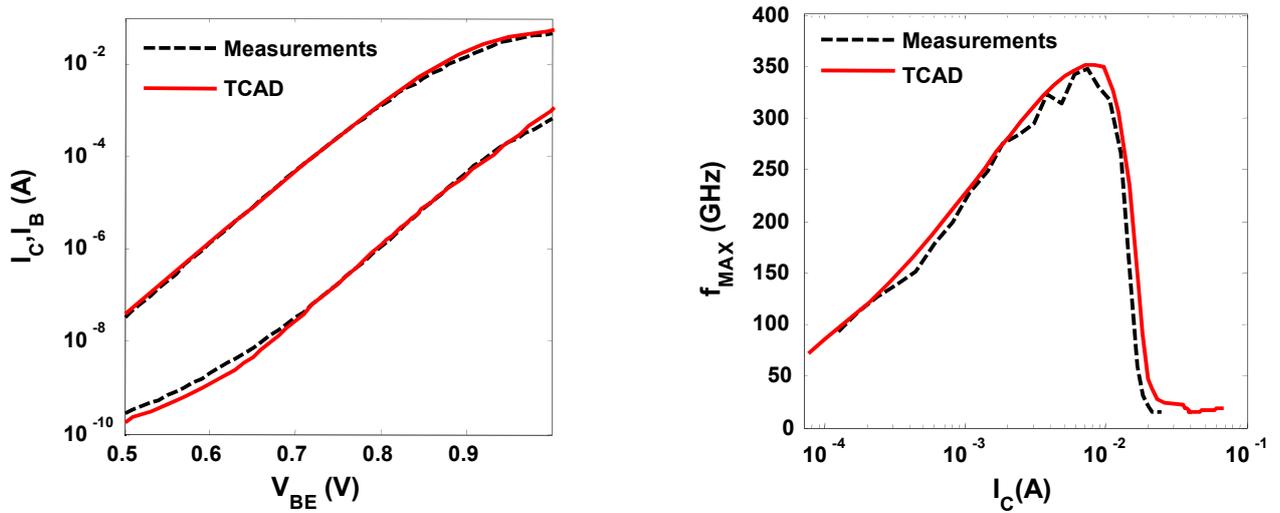


Fig. 3. Comparison with measurement data; (a) Forward Gummel plot at $V_{CB} = 0$ V; (b) Maximum frequency f_{MAX} versus I_C at $V_{CB} = 0.5$ V

SiGeC alloys advanced models simulation allows to model the carbon impact on collector current. Fig. 3, the good correlation between experimental measurement and TCAD simulations allows the validation of simulations.

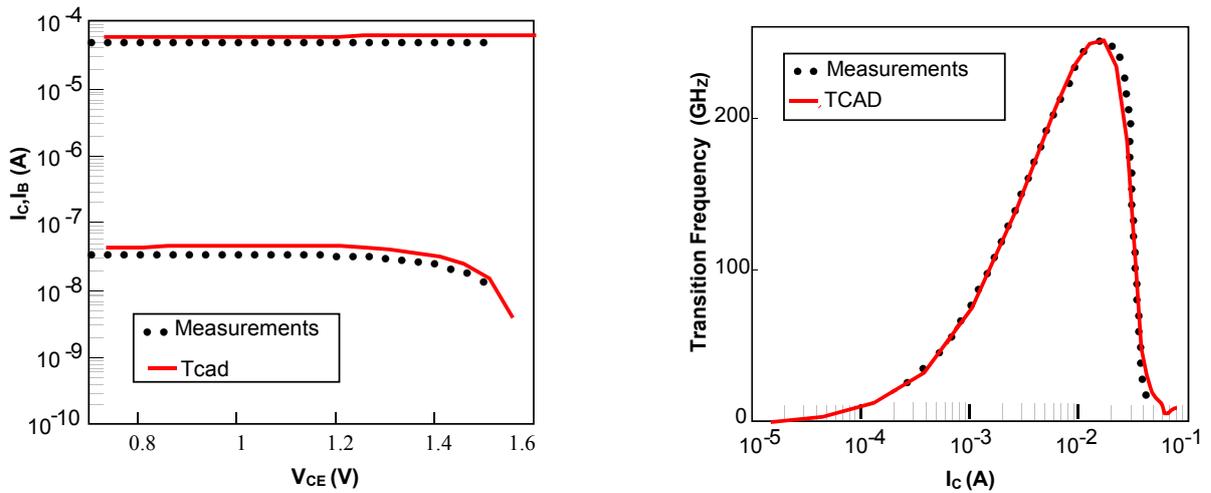


Fig. 4. a) Comparison with measurement data; (a) Collector-emitter breakdown voltage with open base (BVCEO); (b) Maximum frequency of Transition f_T

5. Conclusion

The SiGeC transport models used in our simulations allow considering the influence of Ge and C doping profiles on the electrical behaviour of SiGeC HBT devices. Simulations results indicate that the use of standard transport models for bulk silicon can induce significant errors on electrical characteristics of HBT SiGeC devices. The use of advanced transport models for SiGeC HBTs in TCAD simulation should help to obtain more physical and realistic results, better understanding of charge transport in the device, and facilitate HBT device development and optimization.

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7. References

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