PHYSICAL MODELING OF SEMICONDUCTOR DEVICES FOR MICROWAVE APPLICATIONS

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Abstract

We identify and present important capabilities for the simulation of semiconductor devices, especially in context of the development of microwave applications. The features and their implementational aspects in a simulator are described. Examples are given in order to demonstrate the current abilities of device simulation.

Introduction

Tools for Technology Computer Aided Design (TCAD) have been essential for the development of more advanced and sophisticated devices. In the area of device simulation, the commercial market for simulators is dominated by two companies, Integrated Systems Engineering (ISE) and Synopsis, which are developing DESSIS-ISE [1] and MEDICI/DAVINCI [2, 3], respectively. Silvaco with the ATLAS framework [4] is the third relevant vendor at this moment.

In addition, several academic institutions are developing numerical simulation codes. The spectrum is very large ranging from tools with a small set of highly-specialized features, e.g., PC1D [5], to complete and released simulation programs. An example of the latter category is MINIMOS-NT [6], which has been developed at our institute for more than twelve years as a successor of the well-known Minimos [7]. MINIMOS-NT is a general-purpose, multi-dimensional device and circuit simulator.

Microwave applications must often be seen in a circuit related context [8]. For that reason, circuit simulation programs such as Spice [9], Agilent's ADS [10], or Synopsis' HSpice [11] are employed. Whereas these circuit simulators are based on compact models, also the device simulators with distributed modeling (solving of a PDE system) of the transistors offer so-called mixed-modes. Realistic dynamic boundary conditions imposed by a circuit allow to extract circuit-related figures of merit. Although this approach is limited by performance and memory considerations, the highly sophisticated models required for today's advanced device structures can be directly employed for transient or small-signal circuit simulations [12, 13]. In this work we want to single out these approaches in order to emphasize the device simulation features.

It is a well-known fact, that correct steady-state modeling is an important prerequisite for any kind of subsequent simulations. Thus, the advanced simulators incorporate drift-diffusion and advanced transport models such as energy transport models [14] and provide several advanced mobility models. In addition, models for recombination, band-gap narrowing, impact ionization, band-to-band tunneling, hot carrier injection, Schottky contacts, and floating gates have to be included to account for the properties of advanced device structures.

In the following we identify the small-signal features expected from the simulators for microwave applications. Implementation aspects of MINIMOS-NT and an overview about commercial simulators are given. Examples are shown to demonstrate the current abilities of MINIMOS-NT.

Two-Port Parameters

The major results of a linear small-signal mode are normally sets of two-port parameters used in two-port theory, which are required to describe the performance and properties of a two-port network, e.g. a transistor.

In microwave design the scattering (S-) parameters are preferred because of their measurement advantages. These parameters are related to the traveling waves which are scattered or reflected as the network is embedded into a transmission line of a certain characteristic impedance Z_{L}. Thus, in contrast to the Y-parameters, no short circuit is required which often causes unstable devices and prevents measurements. S-parameters are analytically simple, and provide detailed information on the linear behavior of the two-port.

One has to differ between intrinsic and extrinsic parameters. Basically, the properties of a device are described by the intrinsic parameters, but due to the para-

sitics introduced by the measurement set-up, extrinsic parameters are measured. By means of a small-signal mode, the intrinsic parameters can be simulated and analytically transformed to alternative parameter sets such as S-, Z-, ABCD-, and H-parameters. Hybrid (H-) parameters are often used for the description of active devices such as transistors. Like Y-parameters, they are difficult to measure at high frequencies. The h_{21} parameter is used to characterize f_T, where the current gain has dropped to unity. ABCD- (chain-) parameters are particularly useful for cascaded circuit topologies, since these parameters allow matrix multiplications of the single elements. Measurements of impedance (Z-) parameters require (analogously to Y-parameters) open circuit connections which may act as short circuits at microwave frequencies due to stray capacitances. In addition, an equivalent circuit model of the parasitics can be employed in order to transform the intrinsic parameters to extrinsic ones.

Advanced small-signal analysis modes are based on the S^3A approach presented in [15]. After a conventional steady-state step at a given operating point the simulator is switched to the simulation mode in the frequency domain. The device is excited by a complex-valued sinusoidal perturbation of infinitesimal amplitude. For example, the electron current continuity equation can be symbolically given as:

$$F(V,n,p) = \mathrm{d}G(n(t))/\mathrm{d}t, \tag{1}$$

with nonlinear functions F and G. The time-dependent vector function of electron concentration $n(t)$ is then substituted by

$$n(t) = n_0 + n \cdot e^{j\omega t}. \tag{2}$$

The system is thus Fourier transformed ($dt \rightarrow j\omega$) and the final small-signal approximation is obtained by terminating the Taylor series expansion after the linear part. In comparison to transient methods [16] performance is better (only one equation system per frequency step has to be solved) and the results are more accurate since approximations are not required.

Numerics

Because this approach requires the ability for assembling and solving complex-valued linear equation systems, modules with the respective features have to be employed [17]. There are several approaches for solving these systems: one option is to split the assembled linear equation system $[\mathbf{J}_R + j \cdot \mathbf{J}_I] \cdot \mathbf{X} = \mathbf{B}$ (with $\mathbf{J}_R$ as the dc Jacobian, $\mathbf{J}_I$ as the ac contributions, $\mathbf{X}$ as the complex-valued solution and $\mathbf{B}$ as the complex-valued right-hand-side vector) and the real- and imaginary part is solved separately:

$$\begin{bmatrix} \mathbf{J}_R & -\mathbf{J}_I \\ \mathbf{J}_I & \mathbf{J}_R \end{bmatrix} \cdot \begin{bmatrix} \mathbf{X}_R \\ \mathbf{X}_I \end{bmatrix} = \begin{bmatrix} \mathbf{B}_R \\ \mathbf{B}_I \end{bmatrix} \tag{3}$$

In terms of performance and memory consumption this approach has, especially for three-dimensional simulations, severe disadvantages due to the fourfold-sized system matrix. As stated in [15], the computational effort required for factorization can be excessive. Although iterative methods like block-Gauss-Seidel or block-SOR are suggested for reducing this effort, another approach allows to avoid the split-up. As implemented in MINIMOS-NT, the solver module with its standard iterative solvers can directly handle and solve the complex-valued systems.

Since the measurement considerations are not relevant for numerical simulators, they normally take advantage of the mathematical representation of admittance (Y-) parameters of the linearized device. Because of $Y = I/V$, the contact current I is equivalent to Y in case $1V$ is applied to the contact. If this is done for all contacts, a multiple right-hand-side feature of the numerical tool saves effort, because the factorization of the unchanged system matrix has to be done only once. The accuracy of the calculation can be checked by applying Kirchhoff's laws [18]. In addition, in the case of a frequency stepping, only the complex-valued part of the system is changed.

Extrinsic Parameters

By using a standard two-port pad parasitic equivalent circuit the intrinsic parameters can be transformed to extrinsic ones. Since the elements of this circuit are not exactly determined or measured, an optimization can be performed to calibrate the simulator for a certain measurement equipment (some equipments do this transformation already), which can be completely done in a post-processing step. By varying the free parameters, the error between the simulated and the measured parameters can be minimized.

Additional Figures of Merit

Based on the simulation of two-port parameter sets, additional figures of merit can be deducted. One of the most important figure is the cut-off (transit) frequency f_T, which is defined as the frequency at which the small-signal current gain $|h_{21}|$ rolls off to unity (equals 1 or 0 dB). f_T determines the maximum switching frequency which is very important for digital applications (short ac wise output). This definition assumes the transistor behavior like a single pole low-pass with a slope of -20 dB per decade, which is normally valid, although care has to be taken in respect to very high frequencies. Measurements take advantage of this behavior, since f_T is determined by extrapolating after one frequency point higher than the -3 dB frequency was measured. Since numerical simulators again are not restricted by measurement limitations, the cut-off frequency of the transistor model can be directly determined.

Although a numerical simulator is able to directly and accurately determine the cut-off frequency f_T of the modeled transistor, the performance can be still low. Thus, ways to speed-up such simulations have to be

considered. As stated above, the f_T of a bipolar transistor is characterized as the frequency at which the the ratio $\beta = I_C/I_B$ becomes 1 while I_C (or V_B) is stepped. Hence, two stepping variables are necessary to obtain f_T: for each operating point given by I_C the frequency is stepped until $\beta = 1$. There are several approaches for the frequency stepping: The frequency can be simply increased as long as $\beta > 1$. Then, an interpolation algorithm is used to obtain f_T. Alternatively, the frequency can be increased until the -20 dB slope is reached (or it is used one point only at all) and extrapolation yields f_T. A third possibility resolves the trade-off between accuracy and performance: a conditional stepping based on the Regula Falsi (False Position) can determine f_T after a few frequency steps with a certain accuracy. Since the iteration converges faster to the zero point in the case of narrower boundaries, they should be adapted during stepping giving another performance speed-up.

For analog operations, the maximum oscillation frequency f_{max} is a more important figure than f_T, since there is no ac wise short assumed at the output of the two-port. f_{max} refers to the maximum available gain MAG. A transistor can generate oscillations as long as MAG is larger than 0 dB.

Simulators and Examples

Silvaco's S-PISCES as part of the ATLAS simulation framework [4] calculates steady-state, small-signal ac, and transient solutions for general non-planar two-dimensional silicon device structures. The related simulator for compound semiconductors is BLAZE2D/3D, which provides a library including also ternary and quaternary materials. The calculated small-signal characteristics are the cut-off frequency f_T, S-, Y-, H-, and Z- parameters, the maximum available gain (MAG), the maximum stable gain (MSG), the maximum frequency of oscillation (f_{max}) and the stability factor.

The multi-dimensional simulator DESSIS-ISE [1] provides related features. The small-signal capabilities are incorporated in the mixed-mode, which supports electrothermal netlists with mesh-based device models and Spice circuit models.

Synopsis' MEDICI [2] (a former Avant! product) is a two-dimensional simulator. MEDICI provides Boltzmann and Fermi-Dirac statistics, including the incomplete ionization of impurities. A small-signal analysis can be performed to calculate frequency-dependent capacitances, conductances, admittances, Y-, S-, and H-parameters. DAVINCI [3] is the related three-dimensional device simulation program with a similar set of features. The approach is also based on [15], including the numerical split of real- and complex-valued part.

The first example is an investigation of a $0.4 \times 12\mu m^2$ SiGe-HBT device structure obtained by process simulation [19]. For dc simulations usually only the active part (base and emitter area, collector contact was moved to the bottom) of the device is required. For that reason the collector area was cut to speed-up simulations due to the reduced grid size. However, with the reduced device structure the important capacitances between collector and substrate C_{CS} as well as between base and collector C_{BC} can not be reproduced. In addition, the correct base and collector resistances are missing. This problem can be overcome either by approximating the missing parts in a linear circuit (faster) or by simulating the complete structure, which is more accurate, but in that example 2.5 times slower. In Figure 1 both options are compared: measured and simulated S-parameters at V_{CE} =1 V and J_C = 28 kA/cm^2 are shown in the frequency range between 50 MHz and 31 GHz.

We calculated the gain g_m and the short-circuit current gain h_{21} in order to extract f_T and f_{max}. Figure 2 and Figure 3 show the comparison of our results and the corresponding measurement data. While the measurement data end at 31 GHz the simulation was extended to frequencies beyond this intersection. The peak of the f_T-curve in Figure 2 corresponds exactly to the frequency at the respective intersection in Figure 3. Figure 2 shows also results obtained by DESSIS-ISE using default models and parameters for comparison.

The second example device is a nominally $1.0 \times 8.0\mu m^2$ InP/InGaAsP DHBT self-aligned device structure [20]. The InGaAs emitter cap is followed by an InP emitter and an $In_{0.53}Ga_{0.47}As$ C-doped base at 2×10^{19} cm^{-3}. A quaternary graded spacer is used to connect the base and the collector. See Fig. 3 for a comparison of simulated and measured f_T at $V_{CE} = 1.1$ V and V_{BE} stepped from 0.76 V to 0.97 V [21].

Conclusion

The important features for simulators employed for the development of microwave applications have been identified. The small-signal capabilities of MINIMOS-NT, as basically provided also by the commercial simulators, were demonstrated by current results, including S-parameters, cut-off frequency f_T, and the maximum oscillation frequency f_{max}.

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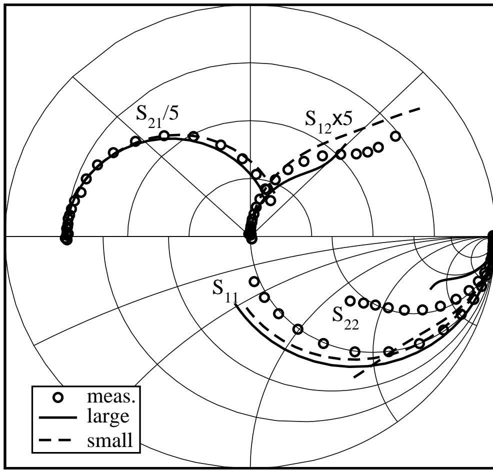

Figure 1: S-parameters of the SiGe-HBT in a combined Smith/polar chart from 50 MHz to 31 GHz at $V_{CE} = 1\,V$ and current density $J_C = 28\,kA/cm^2$.

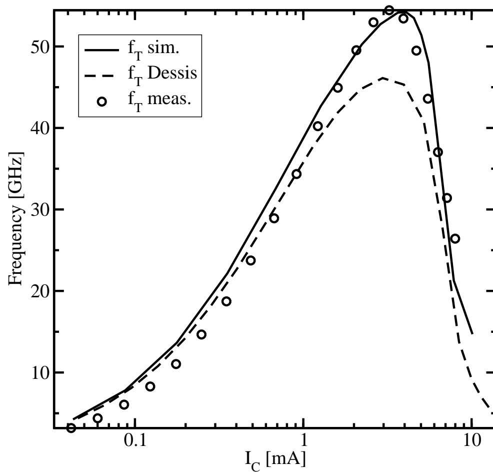

Figure 2: Cut-off frequency f_T versus collector current I_C at $V_{CE} = 1\,V$ for the SiGe-HBT.

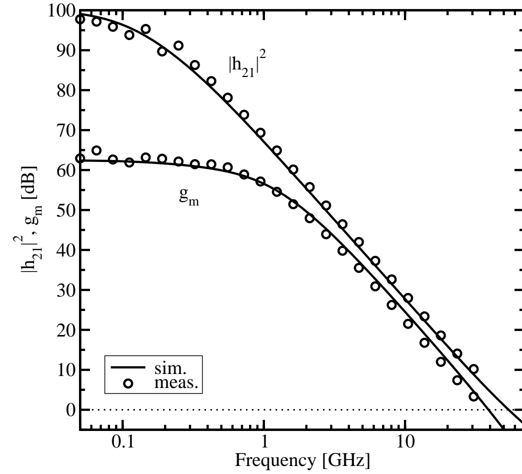

Figure 3: Short-circuit current gain h_{21} and matched gain g_m vs. frequency at $V_{CE} = 1\,V$ and current density $J_C = 76\,kA/cm^2$ for the SiGe-HBT.

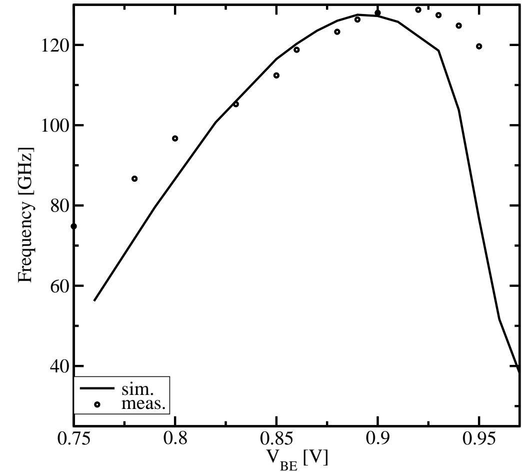

Figure 4: Comparison of simulated and measured f_T curves for the InP-DHBT at $V_{CE} = 1.1\,V$.

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