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# TCAD and EM Co-Simulation Method to Verify SiGe HBT Measurements up to 500 GHz

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## Abstract

A systematic method for the verification of high frequency measurement (up-to 500 GHz) of silicon germanium heterojunction bipolar transistor (SiGe HBT) is proposed. First of all, the method involves an accurate estimation of the effects of passive environment on the overall measurement by a detailed electro-magnetic (EM) simulation. This ensures that the complete measurement environment like probes, pads and access lines along with the appropriate layouts are precisely included in the EM simulation framework. In order to additionally include the active device like *SiGe* HBTs, technology computer aided design (TCAD) tool is used to simulate the device *S*-parameters. TCAD simulation results are fed into an EM-plus-SPICE simulation framework to emulate a complete on-wafer measurement environment. The final simulation results show appreciable correlation with the on-wafer measurement data up-to 500 GHz.

*Keywords:* SiGe HBT, HF *S*-parameter measurement, on-wafer, TRL calibration, de-embedding, TCAD-EM co-simulation, Virtual measurement.

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## 1. Introduction

A reliable circuit design requires accurate compact model of devices to be deployed in VLSI tools. The physics-based models that are used in VLSI tools are highly dependent on accurate DC and RF characterization. Hence it is important to understand the *S*-parameter characterization in high frequency range and verify the models in VLSI tools in that range. But the characterization above 110 GHz is still a challenge and there is no established de-embedding method above this range [1]. In fact, a very few research groups have published *S*-parameter measurement results above 110 GHz [2] [3] [4] [5] [6].

High frequency measurements require careful calibration procedures. Off-wafer calibration is more popular in the production environment [6]. However, since the calibration substrate is different from that of the desired wafer to be characterized, the off-wafer calibration

leads to systematic errors, which is correlated to different probe-to-substrate electromagnetic coupling [7][8]. Similarly, as different probes are used to measure different frequency bands, discontinuity appears in the measured data due to change in RF probes if the probe's cross-talk is not fully corrected by the calibration procedure. A detailed explanation of the work has been reported in [8].

On-wafer calibration is a better choice for high frequency (HF) measurement because it avoids some of the above mentioned limitations observed in off-wafer calibration. Thru-Reflect-Line (TRL) calibration algorithm is the method of choice [2] since it provide a well-defined reference plane and does only require a low knowledge of the standards (geometrical dimensions and characteristic impedance extraction), that indeed gives a better accuracy in the high frequency domain. Nevertheless, this method is not the good choice for the

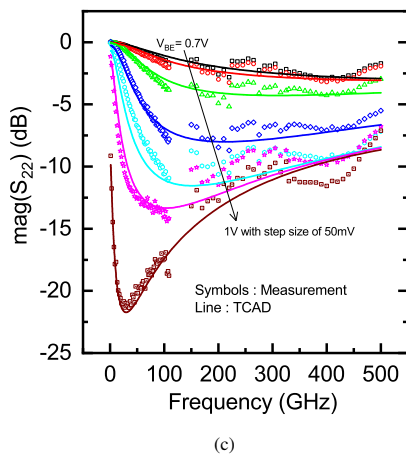
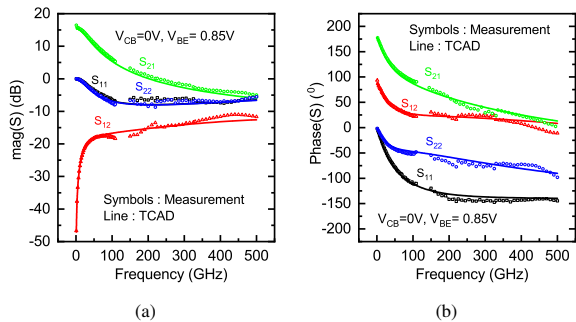


Figure 1: Frequency-dependent (a) magnitude, (b) phase of  $S$ -parameters for the SiGe HBT corresponding to ST Microelectronics B55 process at  $V_{CB}=0V$  and  $V_{BE}=0.85V$ : comparison between actual measurement and TCAD simulation and in (c) magnitude  $S_{22}$  is expanded with  $V_{BE}$  variation at  $V_{CB}=0V$ .

lower frequency since it would require extremely long lines and SOLT/LRM method are more suitable in this low range of frequency.

But while probing the Thru and Line, it is necessary to shift one probe which may add errors in the measurement particularly in case of manual probe stations [4][9]. The drawback of the on-wafer calibration is the need for a specific design of test structure which can be time-consuming. This design requires engineering effort and expertise. For example, the line lengths need to be chosen properly to cover the required frequency band; the geometry of the line needs to minimize the loss and allow only one mode to propagate; the design of the pad itself needs to be optimized to limit the probe-to-substrate coupling; the pad-to-pad distance needs to be sufficiently long in order to ensure a reduced crosstalk and finally one has to keep enough space between the structures to avoid coupling [8][10][11].

In order to check the trend, consistency and accuracy

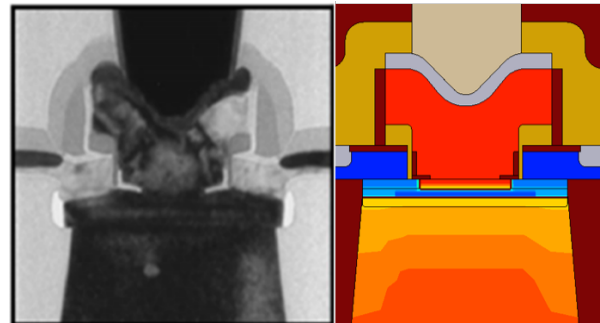


Figure 2: TEM picture (left) of SiGe HBT and corresponding simulated TCAD structure (right).

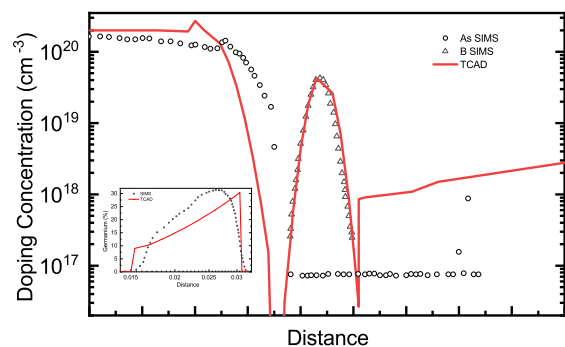


Figure 3: Vertical doping profiles: SIMS profiles of As and B doping (shown in different symbols) and corresponding analytic profile (line) incorporated in TCAD. Inset shows the Ge mole-fraction measured by EDX (symbol) and one used in TCAD (line).

of the high frequency measurement results, one has to compare the data with those obtained from calibrated simulation. One can think of options like TCAD simulation or electrical compact model simulation for this purpose. We have chosen TCAD simulation as reference in this work.

In this paper, using Sentaurus TCAD and Ansys-HFSS electro-magnetic (EM) simulations, we explore and verify the high frequency measurements of SiGe HBTs. As a motivation for such an investigation, Fig. 1 (a) and (b) compares the measurement and calibrated TCAD simulation of frequency-dependent  $S$ -parameters corresponding to a SiGe HBT from ST Microelectronics B55 technology at a particular bias in the main operating regime, and to highlight the deviations magnitude of  $S_{22}$  is plotted w.r.t bias variation in Fig. 1 (c). It is observed that in the lower frequency range (below 110 GHz), the measurement and simulation are in good agreement. However, some discontinuities are observed in the measurement data at the cross-over points (110 GHz, 220 GHz and 325 GHz)

of different frequency bands. Also the characteristics in the upper frequency range tend to deflect from the TCAD simulations. This motivates us to emulate a more realistic measurement environment. To do so, we combine our TCAD simulation results with EM simulation that includes the back-end-of-line (BEOL) along with the probes. This TCAD plus EM simulation data together will be henceforth called as *Virtual measurement* throughout the paper. After that, we follow all the on-wafer calibration and de-embedding procedures on this virtual measurement data. Finally for verification, both TCAD and de-embedded virtual measurement data are compared with actual measurement results.

Section 2 of this paper provides a comprehensive discussion on the calibration of TCAD simulation. In section 3, a brief description of the measurement setup and procedures are provided. The methodology of combining TCAD and EM simulation to produce virtual measurement results is explained in section 4. Finally, we conclude in section 5.

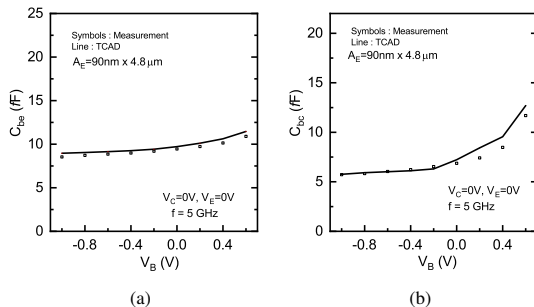


Figure 4: Base-emitter voltage dependent (a) base-emitter capacitance ( $C_{BE}$ ) and (b) base-collector capacitance ( $C_{BC}$ ): comparison between actual measurement and TCAD simulation.

## 2. TCAD Simulation Setup and Calibration

In commercially available Sentaurus TCAD simulator an SiGe-HBT structure corresponding to ST Microelectronics's B55 process is developed as shown in Fig. 2. All the dimensions including the shallow and deep trench isolation are ensured to be closely identical with those of the B55 process during the device design. The doping profiles have been reproduced using analytic mathematical models as shown in Fig. 3 [12][13]. All necessary physical effects are taken into account in the simulation using appropriate models and parameter sets are appropriately tuned from Monte Carlo simulation as discussed below [14][15].

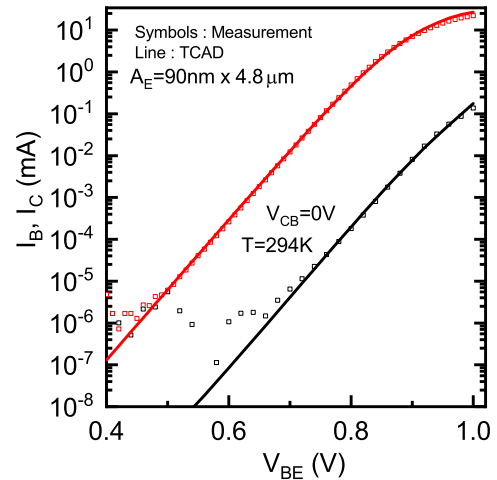


Figure 5: Measured and TCAD simulated Gummel characteristics for  $90 \text{ nm} \times 4.8 \mu\text{m}$  SiGe HBT at  $V_{CB} = 0 \text{ V}$ .

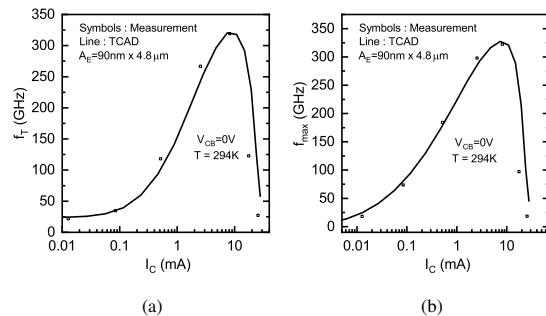


Figure 6: Collector current dependent (a) transit frequency ( $f_T$ ) and (b) maximum oscillation frequency ( $f_{max}$ ) at  $V_{CB} = 0 \text{ V}$ : comparison between actual measurement and TCAD simulation.

For the carrier transport, we have used hydrodynamic model that solves drift-diffusion equations along with the additional energy balance equations for minority carriers. The Sloopboom bandgap narrowing model with appropriately tuned  $N_{ref}$  value is used to account for the effect of carrier concentration at heavy doping [16]. Parameter in the Caughey-Thomas model has also been tuned as suggested in [16]. Shockley-Read-Hall and Auger recombination models are used to take care of the recombination effects and Lackner's model has been considered to include the effect of breakdown at high electric field.

The base-emitter and base-collector junction capacitances, shown in Figs. 4(a) and (b) respectively, are obtained from simulation at low-frequency and are matched with the corresponding measured data to validate the approximation used to emulate the doping profile in TCAD [17]. A maximum permissible error of

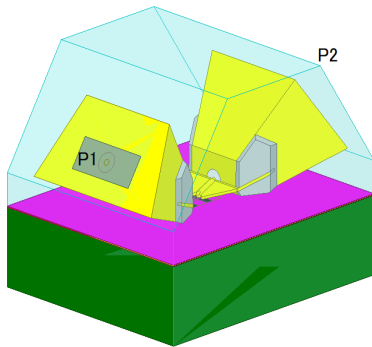


Figure 7: Side view of the EM simulation setup for probes enclosed within an air-box. P1 and P2 probes are marked which are a part of 4-port EM simulation.

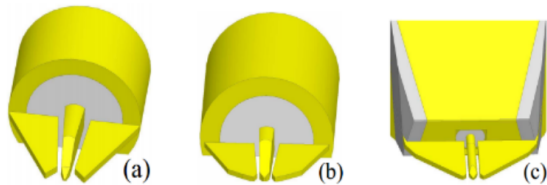


Figure 8: Probe geometry used for different frequency bands: (a) 1-110 GHz (b) 140-220 GHz (c) 220-325 GHz. [20]

0.5 fF is allowed while fitting the capacitances. The recombination parameter in poly-silicon emitter has been tuned to match the base current. A more ideal germanium profile is considered keeping the maximum mole fraction within the permissible range. This effectively helped us in capturing the collector current in the Gummel plot as shown in Fig. 5.

Further, the TCAD simulated transit ( $f_T$ ) and maximum oscillation frequencies ( $f_{max}$ ) are compared with the measured data at  $V_{CB}=0$  V and  $T=294$  K in Figs. 6(a) and (b), respectively, prior to carry out the  $S$ -parameter comparison [18]. It is to be noted that for the  $f_T$  and  $f_{max}$  extraction, a spot frequency at 63 GHz has been chosen [19].

Since the Gummel (Fig. 4) and  $f_T$  characteristics (Fig. 6(a)) show high level of correlation between the TCAD and measured data and since these two characteristics are highly dependent on the intrinsic part of the HBT, one can conclude that a reasonably accurate calibration of the 1D profile of the device has been obtained in TCAD [21]. Since  $f_{max}$  is dependent on  $f_T$  and other external parameters such as base resistance and base-collector and collector-substrate capacitances, the high level of agreement between the TCAD and measured  $f_{max}$  characteristics ensures that the profile parameters

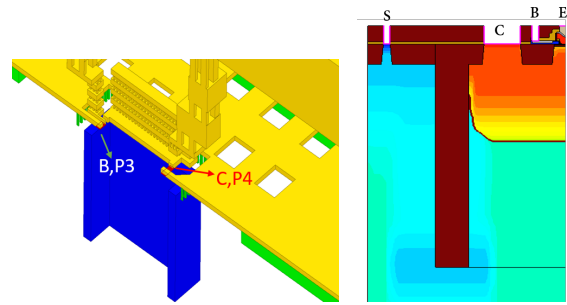


Figure 9: Half structure from EM simulation (left) depicting the other two ports P3 as Base and P4 as collector, below which the active device starts. S, C, B and E in the TCAD structure (right) corresponds to Substrate, Collector, Base and Emitter contacts respectively.

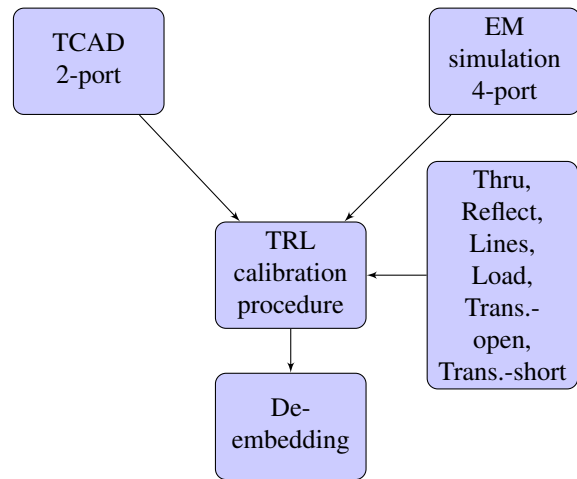


Figure 10: TCAD-EM co-simulation flow leading to a virtual measurement.

related to the extrinsic base, buried layer in the collector region and the substrate doping at its contact and around the deep trenches are closely identical with those of the B55 process. The same is also confirmed from  $S_{22}$  parameter shown in Fig.1 (c).

This is also validated after looking into the doping profiles received from ST Microelectronics (not disclosed here due to intellectual properties agreements).

### 3. Actual Measurement Procedure

We have carried out the  $S$ -parameter measurements up-to 500 GHz for  $V_{BE}$  varying from 0.7 V to 1 V and  $V_{BC}=0$ V. In order to measure from 1 GHz to 500 GHz, four different measurement benches such as (i) Agilent's E8361A VNA up to 110 GHz using extenders (N5260-60003) above 67 GHz (ii) 140-220 GHz (iii) 220-330 GHz and (iv) 325-500 GHz bands with a four-

port Rohde & Schwarz ZVA24 VNA coupled with extenders (ZC220-ZC330-ZC500) have been used. The power level is set to approximately -32 dBm using a calibration table provided by extender supplier in the four bands for measurement of both active and passive elements (the latter are used for de-embedding purposes). Picoprobe RF probes with  $50\ \mu\text{m}$  pitch are used for covering the bands above 110 GHz and  $100\ \mu\text{m}$  pitch probes are used below 110 GHz. On-wafer TRL calibration and standard Short-Open de-embedding has been performed. The reference plane of the TRL is set at the top metal and at sufficiently close proximity of the vias. In the subsequent de-embedding step, which can be performed according to the well-known "lumped element" approach, only the via stack has to be removed.

#### 4. Virtual Measurements, Results and Discussion

As discussed in section 1, after observing a mismatch between the actual measurement data for  $S$ -parameters with calibrated TCAD simulation, we decided to include the non-ideal environment factor related to BEOL, pad-parasitics, probes etc. into the TCAD simulation results via additional EM simulation. For this purpose, we performed three-dimensional (3D) EM simulations using commercially available simulator, *Ansys-HFSS*. The simulation layout is imported on a silicon substrate and the probes are placed approximately the way they appear during the measurement [20]. Then, the whole structure along with the probes is covered within an air box as shown in Fig. 7. During the setup, proper care has been taken in choosing the meshing and assigning the appropriate boundary conditions for absorbing the radiation at the faces of the air box in order to emulate an infinite free space environment. Three separate probe models for each frequency band as shown in Fig. 8 are chosen and finally simulations are performed by giving input excitation at each wave-port. Together, the TCAD simulation of SiGe HBT up to Metal-1 and the EM simulation to account for the remaining non-ideal environmental factors, as described above and shown in Fig. 7, Fig. 8 & Fig. 9 generate the virtual measurement data for our further investigations.

Now we compare actual measured  $S$ -parameter results with (i) TCAD simulation (of the actual device up to metal-1) and (ii) virtually measured data. Virtual measurement data are achieved following the flow graph described in Fig. 10. First, the RF probes, the pads and the BEOL down to metal 1 where the transistor is connected, are simulated with HFSS (4-port EM simulation). Next, the TCAD (2-port TCAD) and EM

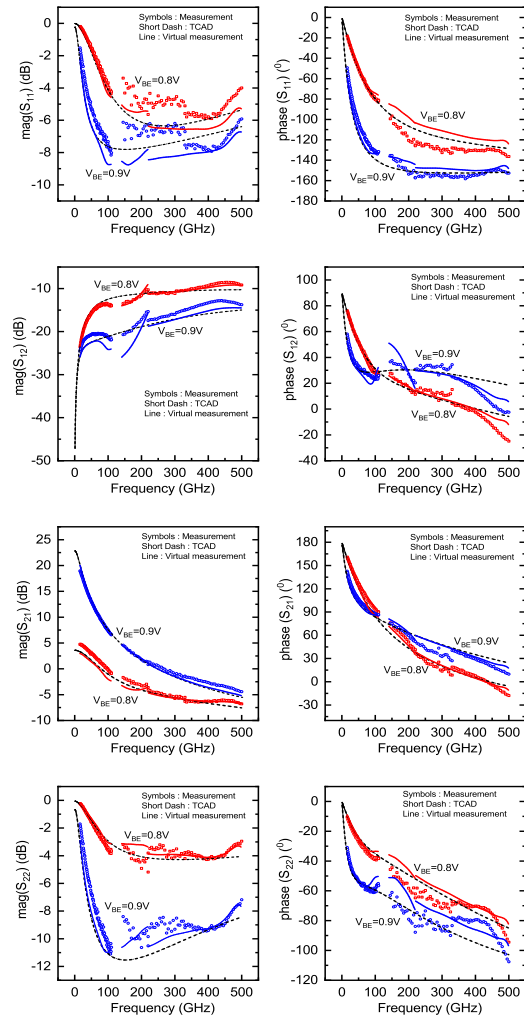


Figure 11: Frequency dependent magnitude and phase of  $S$ -parameters at  $V_{CB}=0\ \text{V}$  and  $V_{BE}=0.8\ \text{V}$  and  $0.9\ \text{V}$  for the SiGe HBT up to metal-1: comparison of de-embedded actual and virtual measurements with TCAD simulation.

simulation results are concatenated. This data set contains both the access (probes, pads, BEOL) as well as the actual transistor itself. The next step is to perform a calibration and de-embedding as done in real measurement. For that purpose, all TRL calibration standards are simulated with HFSS and the calibration is performed as shown in Fig. 10 [22]. Finally, the Short-Open de-embedding structures are simulated as well and the de-embedding is completed leading to the virtual measurement data. If calibration and de-embedding had been ideal, the de-embedded virtual measurement data would perfectly match with the TCAD simulation of the actual transistor. The results for the three data sets (actual measurements, TCAD simulation and vir-



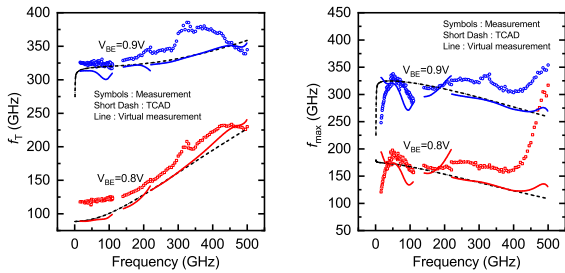


Figure 12: Frequency-dependent transit frequency ( $f_T$ ) and maximum oscillation frequency ( $f_{max}$ ) at  $V_{CB}=0$  V and  $V_{BE}=0.8$  V and 0.9 V for the SiGe HBT up to metal-1: comparison of de-embedded actual and virtual measurements with TCAD simulation.

tual measurements) are compared in Figs. 11 and 12 for the magnitude and phase of  $S_{11}$ ,  $S_{12}$ ,  $S_{21}$ ,  $S_{22}$  and  $f_T$ ,  $f_{max}$  up to 500 GHz.

From the comparison plots following observations are made.

- Up to 100 GHz, a good correlation can be observed for both  $V_{BE}$  bias points and for all four  $S$ -parameters (magnitude as well as phase).
- In the frequency range of 50-100 GHz, we can observe there is a sudden reduction of  $f_{max}$ , it can be observed from  $S_{12}$  parameter which is strongly related to  $f_{max}$  and can be attributed to cross-talk. A similar dip is observed in  $f_T$  also in 50-100 GHz range can be due to minor difference in probe angle and position in both real and simulation environment. It can also be observed in magnitude of  $S_{21}$ .
- When changing the frequency bands (especially at the transition into the 140 GHz to 220 GHz band), discontinuities are observed with the actual measurements while comparing with TCAD and virtual measurements. Therefore, it can be concluded that the TRL calibration along with short-Open de-embedding are not able to correct the coupling with HF probes and the wafer surface accurately, for the given test-structure and the HF probes used. Also, the measurements are noisy and can be attributed to some difficulties to have a reliable contact between the probes and pads and in particular considering the small signal pad surface ( $40 \times 25 \mu\text{m}^2$ ) and the thickness of the passivation layer. In fact the very short tips of the WR3.4 probes and their angle does not allow to have a reliable contact on our BICMOS test structures (please note that this is not the case on calibration test structures).

- The discontinuous transition of actual measurements at 220 GHz is well predicted by the virtual measurement especially for the magnitude of  $S_{12}$ -parameter. This discontinuity has already been studied in [20]. WR5.1 (140-220 GHz) uses a technology which is closed to the probe designed for 110 GHz band while the WR3.4 (140-220 GHz) use a very different technology which is much more scaled. We have demonstrated in [20] that the coupling with the environment is much stronger when the EM field is not confined by a highly scaled probe.

- Because of different resistance of bias tees from probe to probe there can be a change in bias current. The bump in the actual measurement data of  $f_T$  characteristics (Figure 12) in 320-420 GHz range can be a due of this resistance difference.

- When going to higher frequencies beyond 400 GHz, a deviation of the expected behavior can be observed both in virtual as well as actual measurements compared to TCAD data. Even though no perfect agreement for the actual or virtual measurement data is achieved with the reference TCAD data, at least the trend is reasonably predicted. We suppose that the cross-talk is the source of this discrepancies since the magnitude of  $S_{12}$  is increasing more than what is predicted by the TCAD. Please note the TRL calibration does not correct the cross-talk. The distance from pads to pads must be increased to reduce this effect. If with the picoprobe 110 GHz with 100  $\mu\text{m}$  pitch the cross-talk start to influence the results above 70 GHz, using a highly scaled probe such as the picoprobe WR2.2, the cross-talk start only above 400 GHz.

This brings us to the conclusion that the calibration and de-embedding procedures are still need to be improved especially at the higher frequency bands and require further improvements in order to correct all the demonstrated errors introduced by the measurement environment. Two roads of improvement for measurement accuracy needs to be explored in parallel, one involving the design of the test structures the other one is about the design of the probes:

- On one side, the design of the test structures already uses a boundless ground plane, a large space between each structures (200  $\mu\text{m}$  in X and 133  $\mu\text{m}$  in Y-direction) may still be improved on the two following points: the distance from pad to pad to

reduce the cross-talk and the design of the pad itself which is mainly empirical. Please note that most of the improvement leads to very costly test structures.

- On the other side, The WR3.4 and WR2.2 probes are highly scaled probes which gives very reasonable results [20] but requires much higher manufacturing cost. If one can develop similar probes design keeping the same geometry scaling but with the connector for the lower frequency band (especially 140-220 GHz), the measurement accuracy would be much improved.

## 5. Conclusion

For the first time, we analyzed a very high frequency (>110 GHz) measurement data using two finite element tools; one solving the EM equations and the other solving the semiconductor equations. The presented methodology provides one with sufficient confidence in the adopted characterization techniques and results. More precisely, it allows one to differentiate between accurate and erroneous characterizations. This work is a step forward (i) to adopt an improved characterization technique and (ii) to validate the TCAD result in high frequency aiding the modeling of non-quasi static and other high frequency effects. As a whole, the analysis outlines a prescription in order to make the researchers aware of certain precautions while designing the test structures, carrying out the process of characterization and verifying the corresponding results. The detailed methodology, if adopted, will certainly help in the accurate extraction of high-frequency compact model parameters.

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