Physics-based simulations are a powerful tool to analyze the behavior of semiconductor devices under different operating conditions. Due to the continued shrinking of transistor dimensions, the scenario of semiconductor device technology is nowadays characterized by the significant technological variability and difficult thermal management, strongly affecting the device operation and producing a spread of their performances. Physics-based sensitivity analysis is the ideal tool to link physical/technological parameter variations to the device performance spread, but its numerical burden may prove to be a limiting factor in the widespread diffusion of TCAD tools, especially in frequency-dependent multi-harmonic analyses. One way to overcome this limit is to rely on new agile and flexible techniques, such as the Green's Function (GF) approach.

This thesis presents the framework of advanced physics-based modeling for the peculiar needs of microwave devices. An in-house, pre-existing 2D physics-based simulator, allowing for large-signal multi-tone periodic and quasi-periodic analysis through the Harmonic Balance technique, has been extended and optimized. The original version of the in-house code, implementing the drift-diffusion model, has been improved through the treatment of more accurate temperature dependencies in the most important materials, e.g. Silicon, GaAs, GaN. The worsening of environmental conditions makes thermal management increasingly important, leading to the need of implementing the self-heating equation. The investigation of trap signatures, another fundamental aspect to achieve good RF performances, has been accounted implementing the trap rate equation. These advanced capabilities make the in-house simulator able to evaluate frequency dispersion effects related to temperature and trapping mechanisms, also including an interplay of traps and thermal dynamics. Moreover, the TCAD solver has been extended to allow for efficient sensitivity analyses in both static and dynamic conditions through the GF technique, with the aim of assessing the device response to a small physical/technological parameter variation, e.g. temperature, doping concentration, trap energy, etc. These improvements make the TCAD solver very appealing with respect to commercial tools for the simulation of nanoscale devices in analog RF/microwave applications.

The research activity has addressed two significant case studies to demonstrate the TCAD capabilities. A *T*-dependent sensitivity analysis is presented on a 54 nm Si FinFET Class A Power Amplifier (PA) in both the DC case, including self-heating, and the LS regime. The analysis demonstrates the accuracy of the GF technique and its advantage in terms of simulation time of about 20%. Thermal sensitivity affects all operating conditions, showing more than 1 dB output power reduction at T=350 K. LS *T*-dependent simulations are also performed with the concurrent variation of an additional parameter, i.e. load and doping concentration of the source/drain regions. The analyses are carried out with no extra numerical burden and demonstrate that temperature variations dominate over load sensitivity, while concurrent doping variations further affect the PA 1 dB compression point.

The TCAD high computational cost suggests that it cannot be used routinely for circuit design, but it can a basis to extract computationally efficient circuit-level models. As a demonstrator, a complete dynamic electro-thermal analysis has been developed on the same PA exploiting the *T*-dependent X-parameter model, exported from TCAD simulations into EDA tools. The accuracy of the *T*-dependent X-parameter model is demonstrated by comparing circuit simulations with TCAD results in continuous wave, including self-heating. The analysis is extended to pulsed modulated operation, highlighting thermal dynamic effects as a function of the pulse period. Finally, the pulsed operated analysis is repeated for a Class B PA to highlight the different role of thermal memory.

TCAD analysis represents a unique opportunity to investigate the impact of traps in the GaN technology: DC and AC GF-based sensitivity analyses are performed on a 0.150 µm Fe-doped AlGaN/GaN HEMT through to the variation of a trap physical parameter, e.g. trap energy and concentration, showing accurate results with respect to repeated TCAD simulations. Traps are responsible for the low-frequency dispersion peak of the Y-parameters, which is shifted towards higher values with decreasing trap energy level. Furthermore, the GF approach allows to extract the local sensitivity, giving a unique insight into the device operating conditions and showing the parts of the device where traps influence most the HEMT AC parameter.