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Research Article

Fabrication Process Stochastic Model for Yield Estimation in Microwave Semiconductor Devices Production

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This paper presents a new methodology for simulation of production processes in order to determine device parametric yield. The elaborated methodology is focused on capturing stochastic relations between every parameter of the subsequent processes that are impossible to determine directly. The current state-of-the-art together with the gaps in the knowledge regarding yield modelling is presented. A novel approach to the important issue of effective yield modelling that allows the overcoming of current challenges is presented. The methodology's usefulness is validated with the example of the fabrication process of AlGaN/GaN HEMT (high electron mobility transistor) for application in high-frequency electronics. Fabrication of AlGaN/GaN HEMTs is a complex process due to the large number of technological stages required, most of which are still the subject of ongoing research. Most importantly, the approach presented in this paper could be easily applied to the modelling of any complex production process in every case where it is necessary to examine relations between the final product parameters distribution and the values of the involved process parameters.

1. Introduction

The characteristic feature of the semiconductor devices manufacturing industry is multistage, inflexible processes, which demands sophisticated and high-cost equipment and utilizes expensive materials. Although demanding, the industry is important economically. The size of the global market for semiconductor devices in 2016 reached 339 billion USD with further projected growth dynamics in 2017 of 11.5%. An additional trend that impacts its operation is a constant decrease in capital margins. Thus, every possible means of cost reduction should be explored and applied for developing and protecting the competitive advantage of a company. Essential for reaching this goal is the incorporation into the design and fabrication process of semiconductor devices as well as analysis of both parametric and functional yields. This allows for decisions optimization in numerous areas: device design, technology node selection, and the choice of fabrication process parameters values, which should result in the increased economic effectiveness of the developed solution both in terms of production chain optimization and final product margin.

The yield analysis has to be performed comprehensively in every stage of device design and fabrication. Typical methods of yield analysis impede introducing the necessary optimizing changes, due to the large amount of data required, which can be collected only after finishing the fabrication process deployment. The methods usually consist of two stages. In the beginning, results of technological processes are collected, and later, the various statistical models are fitted to the data [1–3]. Unfortunately, the scope of possible changes that can be implemented on the base of the formulated conclusions is rather limited, because of the aforementioned inflexibility of the manufacturing cycle. The visible need for faster knowledge implementation regarding the predicted device yields in the design of the semiconductor, and their fabrication process constitutes the main research motivation of this paper. In the presented paper, the elaborated model of the semiconductor device fabrication process is presented elaborated on the experience of academic research, and development laboratory involved in the design and fabrication of modern devices based on compound semiconductors. The model described below enables the simulation of the whole process starting from separated procedures. It was applied to analyze the parametric yield of AlGaN/GaN HEMT dedicated for high-power RF switching at C (4–8 GHz) and X (8–12 GHz) bands. AlGaN and GaN are nitride alloys of metals from the third group of the periodic table (respectively, aluminium and gallium). They are widely used in the semiconductor industry, due to their unique combination of features: high-temperature conductivity, wide and straight bandgap as well as the occurrence of piezoelectric effects.

The main objective of the performed research was to establish the statistical distribution of transistor drain current in production batches. Particularly important was the determination of the impact of an early stage technological process–namely the selection of AlGaN/GaN HEMT-type heterostructures grown by the MOCVD (metal-organic chemical vapor deposition) technique on the sapphire substrate. The knowledge of the statistical distribution of transistor drain current in production batches is essential for cost reduction and yield increase.

It is obtained by eliminating wafers with deposited heterostructures whose parameters do not guarantee the fabrication of devices with expected parameters. Moreover, the developed approach enables the comprehensive description of available knowledge, including all involved areas: applied technology, device design, element design, characteristics of specific equipment, process parameters, applied materials and reagents, measurement methods, environmental influence, as well as the staff's knowledge, experience, and their individual learning curves. An additional advantage is the possibility of incorporating this analysis early, during the design phase or even during the selection of the technology.

2. Yield Analysis Methods

In the literature concerning semiconductor manufacturing, few kinds of yield are specified along with different phases during production when being measured [4]. The main division lies between functional and parametric yield. Former called catastrophic yield is considered fundamental and most widely used, due to the advanced mathematic theory of its description. In basic terms, the functional yield for a given manufacturing process is defined as the ratio of good elements at the output stage of the process to the number of elements at the input. In the case of AlGaN/GaN high-electron-mobility transistors (HEMTs) fabrication, a list of main processes includes cleaning procedures, epitaxy, lithography, etching, and metallization deposition, and their electrolytic thickening, passivation, to the separation and packaging of the whole chips. To conclude, the functional yield is a scalar measure of process efficiency. From a single yield of respective processes, denoted y_{n}, one can determine the yield, Y, of the whole process as

$$Y = \prod_{n=1}^{N} y_n. \quad (1)$$

In general, the single functional yield, y_{n}, is determined by some function f_{n} with parameters A_{c}, D_0:

$$y_n = f_n(A_c, D_o), \quad (2)$$

where A_{c} is the size of the chip critical area and D_0 is the unit defect density. The range of f_{n} functions family is wide and includes different statistical approaches to the described process. Model calibration is performed based on the production data analyses and allows for accurate functional yield prediction of the semiconductor devices and integrated circuits (ICs). Recent research in this area is focused on including mathematical models of learning curves and predictors of stochastic variability in the function, f_{n} [1, 4, 5].

Although it is commonly utilized in various analyses, functional yield due to its specificity has limited applicability. Functional yield is the scalar measure, describing only the percentage of acceptable elements after the single process, losing details of the technology complexity of semiconductor devices fabrication technology, thus providing no information about distributions of the values of their operating parameters. Such information is required to optimize device design and fabrication process in regard to their performance and manufacturing cost.

Measure describing device parameters distribution is the parametric yield that is represented by the probability density functions set of random variables $\{X_{\mathrm{i}}\}$, where any X_{i} represents some output parameter measured either between processes or of the finished device. In the case of AlGaN/GaN HEMT, parameters yield analysis includes distributions of maximal drain current (I_{DSS}), pitch-of voltage U_{p}, cut-off frequency f_{T}, MAG (maximal available gain), and other parameters. Contemporary methods of semiconductor devices and IC parametric yield analysis in most cases utilize elements of big data methods combined with statistic regression models [3, 5, 6]. Complex GLMMs (generalized linear mixed models) are applied, allowing for the description of the nonlinear dependencies between variables. Such an approach, although effective in a production environment, is hard to apply into research and development of device design and technology, due to the limited volume of experimental data available and the high cost of their acquisition. Approach taken in such cases is based on TCAD methods and simulation of respective processes [7–9]. It enables to acquire data regarding specific relations that influence device operation and its parameters distribution without conducting numerous experiments. Though, the limitation of this methodology is challenged by a precise description of relations between parameters in the scope of the whole devices fabrication process. Consequently, due to the complex characteristic of involved relations, there is impossible to develop tools that use purely analytical formulas and capture the stochastic characteristic of modeled fabrication process.

In the frame of the conducted research, the approach was proposed that enables the unification of all aforementioned methods: big data analysis, TCAD simulations, and heuristic observations about respective processes that are based on the experience of the research team, as well as available literature data. This approach fits into methodologies reported in various publications applying big data methodologies including machine learning methods [10, 11]. However, it diverges from this method by focusing on including conclusions based on analysis of small scale targeted experiments. The approach is based on developing a framework that will be capable of capturing all of the involved relations together with correlations between them and efficiently generating possible realizations of such a stochastic model. It fits into the wide scope of Monte Carlo methods. The next performed step is to analyze acquired data with the aim of statistical inference about the influence of respective processes variables on operating parameters distributions in HEMT, during its designing and manufacturing.

3. The Developed Model Overview

In order to analyze the parametric yield of AlGaN/GaN HEMTs, a novel approach was applied. It is based on created from scratch universal simulation software framework that operates on the textual representation of the manufacturing process. The representation includes all important technological processes parameters, results of interprocess measurements as well as ultimate device operation parameters. During the development, a number of assumptions were made, in order to maximize the flexibility of generated predictions. It was necessary, considering the iterative nature of conducted research. They result in an incremental increase of available knowledge regarding AlGaN/GaN HEMTs manufacturing and design. The aforementioned reasons force the initial requirement that in the model all involved parameters can be random variables with arbitrary continuous or discrete distribution, and for a given random variable, it should be sufficient to state solely the arbitrary cumulative distribution function. Furthermore, every input variable can be freely cross-correlated with each other. Regarding the dependent variables derived from model parameters described previously, it will be possible to include them in the model as arbitrary nonlinear explicit functions, whose coefficient can be also stochastic variables. The dependent variables in the model usually are interprocess measurements results or ultimate device parameters. Introduced above described requirement of the possibility to utilize an arbitrary distribution creates challenges regarding the computing complexity of random samples generated by the Monte Carlo method. Though simplification was implemented, every continuous distribution that is nonnormal will be discretized. Possible errors and inaccuracies created by this approach can be neglected, because of the possibility of freely increasing discretization density. It is possible, due to applied search algorithms of the computation complexity of the class O (log n). In Figure 1, the scheme of the proposed model of variables representation illustrating the correlations between them is presented.

The entire novel part of the created methodology is the development of a method to textually represent model parameters. A special XML structure was developed to satisfy this need. Due to this, the main risk for the implementation of the modern design support and knowledge management tools was mitigated, which is extensive IT knowledge required in order to effectively use them. In the developed form, the model can be used and modified by the person without special training.

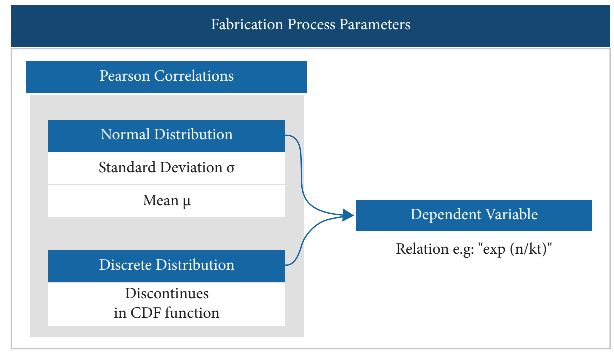

Figure 1: Proposed scheme of variables representation and correlations between them.

Additionally, feedback coupling was predicted between the software part, responsible for samples generation, and the model that can be used for self-calibration as well as for performing statistical Bayesian analysis [12]. The prototype of the software framework was developed using *Python* language and is fully functional allowing for model description loading and transformation into memory objects, generating a stochastic realization of the process, as well as saving and data acquisition. Applied mathematical functions are from the commonly acclaimed scientific computing library SciPi (0.18.1). Essential, for the model application, is an efficient algorithm for model realization generation. It requires using a method capable of generating samples from arbitrary cross-correlated distributions both continuous and discrete.

4. Model Structure

The model is the description of subsequent manufacturing process steps by a number of representative variables, $X_{\mathrm{n,m}}$ whose values are realizations of certain stochastic processes. For example, the expected epitaxy temperature is 800°C; however, the actual temperature of the process is subjected to variability due to mechanical and electrical factors. The distribution of obtained temperatures among the number of processes can be described with Gaussian distribution. The same regards for all of the other parameters. After every step, a number of resultant output parameters, $X_{\mathrm{n+1,k}}$ are generated using arbitrary nonlinear functions of $X_{\mathrm{n,m.}}$ For example, in the case of the epitaxy process, the resulting sheet resistance is calculated from the process temperature described above, together with flows, and composition of reagents. The function relating all involved parameters is nonlinear, and not all input parameters have Gaussian distributions; as a result, obtaining analytical distribution is impossible, although by applying Monte Carlo simulation one can obtain stochastic dependence between variables. Consequently, obtained resultant parameters can become input parameters for the next process steps. Thanks to this, it is possible to analyze a complex multistage production process with a number of branches.

The number of simulation steps is unbounded and allows for the description of the complete manufacturing process. Ultimate results of interest are distributions of dependent variables in the last process step, which represent device operation parameters. Their distribution together with the possibility to calculate correlation with input parameters represents a directly parametric yield of fabrication process and dependence of yield on certain process variable values. Information is presented in the form of a vectors table with exact values obtained in every subsequent Monte Carlo iteration. Such table number representation allows for the description of stochastic relations of every parameter of the subsequent processes that are beyond the analytical composition of normal and discrete distributions. The flow of the algorithm is present in Figure 2.

The proposed methodology allows for observing the dependence between parameters in every moment of the production process. It is a useful tool for parametric yield analysis of devices or integrated circuits. Especially, it enables us to understand the impact of given input process parameters on the distribution of ultimate product parameters.

5. Random Samples Generation from Arbitrary Distribution

An essential aspect that needs to be addressed before the hands-on application of described above model is the efficient generation of random samples from arbitrary both continuous and discrete distributions. Therefore, to generate random variables vector, $\overline{F}$ realizations with covariance matrix ΣX, the NorTA method was applied. Expansion of this name is "Normal to Anything" which illustrates the principle of its operation. The advantage of the method is the ability to generate samples from arbitrary distributions combined both continuous and discrete while preserving the computation efficiency. The only requirement, in order to effectively apply the method, is the existence of an inverse cumulative distribution function [13].

The NorTA method consists of a few steps. In the beginning, a vector of random variables realization is drawn from multivariate normal distribution $N(0, \Sigma_Z)$ with a certain matrix covariance Σ_Z that needs to be previously determined. Furthermore, every generated sample is transformed by the normal cumulative distribution function $\Phi_{(0,1)}$. After this operation, the variables vector of uniform distribution $U(0, 1)$ is obtained. The received relation $\Phi_{0,1}(N_{(0,\Sigma_Z)})$ is a Gaussian copula and preserves initial covariance relations within the input vector. The last step is the transformation of the samples vector by the vector of inverse distributions of desired random variables $\overline{F}^{-1}$. Samples obtained in that way are the realization of that random variables vector with cumulative distribution functions, $\overline{F}$, and cross-correlation matrix Σ_X.

The essential question in effective NorTA algorithm application is the determination of the covariance matrix Σ_Z elements that will result in the generation of the samples vectors with desired correlations. It is a computationally intensive task. Different approaches are applied from the analytical solutions that unfortunately narrow possible combinations of input parameters distribution to the pair of continuous-continues, continuous-discrete, or discrete-discrete to the methods based on the optimization of the nonlinear stochastic functions. In the developed framework, the former was applied, even though more computationally complex, enabling the unified approach to the issue of determining covariance's matrix Σ_Z. Moreover, for a given set of model random variables, the covariance matrix is determined only once for any pair of variables, which does not influence considerably total computation time [14, 15].

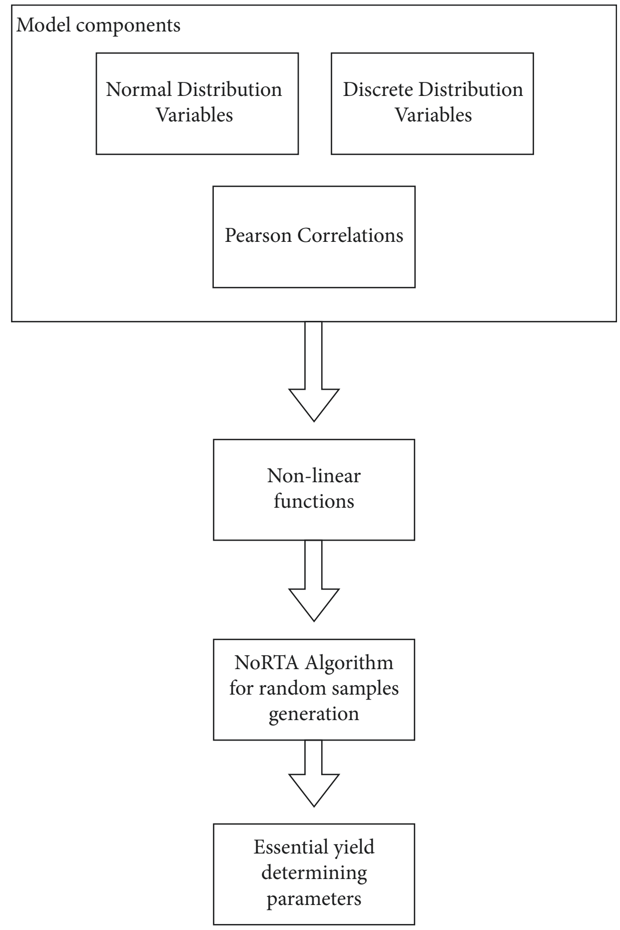

Figure 2: Flow chart presenting the steps used in modelling process.

6. Model Application and Results

The described model was applied to modelling of the AlGaN/GaN HEMT fabrication process. The developed model enables the investigation of arbitrary relations between various parameters of the fabrication process and was aimed at the optimization of the research plan of AlGaN/GaN HEMT dedicated to microwave applications.

AlGaN/GaN HEMTs are essential for both civilian and military markets since they constitute an important part of radars, telecommunication power amplifiers as well as power transforming devices (inverters and converters) [16]. However, the fabrication of such devices is highly demanding in terms of process complexity in comparison with silicon technology. Usually, the process involves several dozen of steps. In general, the first group of processes constitutes an epitaxial deposition of AlGaN/GaN HEMT type heterostructures by the MOVPE technique. Any epitaxy process parameters modifications, such as temperatures, pressures, and reagents content and composition, result in a variation of electric heterostructure parameters and as a result strongly influence the main electrical parameters of these structures, namely two-dimensional electron gas (2DEG) concentration, pitch-off voltage, and surface resistivity. All of the aforementioned heterostructures' electrical parameters could be measured before the fabrication of devices by nondestructive methods and enabled to select the substrates with required parameters. Subsequently, after the growth of the heterostructure, the fabrication processes of the devices start from the Meza structures of the definition of the device performed by lithography and reactive ion etching (RIE), using Cl_2/BL_3-based plasma. Subsequently, process quality control is performed via a range of microscopic measurements, using scanning microscopy (SEM) and atomic force microscopy (AFM). Furthermore, ohmic contacts are fabricated. They are formed by multilayer (Ti/Au/Mo/Au) metallization and must be annealed at a high temperature. Then, in order to control the drain current in the transistor channel, Schottky contact has to be fabricated and placed in the area between the drain and the source contacts. There are two possibilities for its fabrication. The selection of the appropriate method depends on desired gate length. For gates longer than 1 μm, the photolithography technique (PhL) could be used, whereas, for gates of the length between 100 ÷ 500 nm, the electron beam lithography (EBL) technique has to be applied. At our laboratory, two different metallizations were used for Schottky contact: Ru/Au or Ni/Au fabricated by lift-off process of metallization applying PhL or EBL techniques, respectively. At the next stage, the passivation process, using polyimide materials, is conducted, and the transistor is ready. However, manufacturing of consumer available product requires a few more processes, such as the thickening of all metallization, cutting substrate for chips, bonding, packaging, and encapsulation.

At this stage, the range of electric DC and microwave measurements are conducted on the wafer using the specialized probes as, at this stage, it is possible to measure final device parameters. One of the most important is the saturate drain current, I_{dss}, that determines, among others, the suitability of the transistor to switch high RF powers. In Figure 3, the transistor structure operating at X-band (8–12 GHz) is shown.

They were designed and are applied under the frame of the project to develop novel military radar systems, with solid-state devices that could replace the traveling wave tubes (TWT). The C band transistors have the gate length, L_g, equal to 1000 nm, with the width of $W_g = 10 \times 125\,\mu\text{m} = 250\,\mu\text{m}$ fabricated by photolithography, whereas the X-band transistors have the gate length of the range from 100 nm to 500 nm with $W_g = 2 \times 125\,\mu\text{m} = 250$ mm fabricated by electron beam lithography.

The developed model was applied to combine results of the number of discrete research on subsequent technological steps in a coherent way that allow the prediction of operating parameters of obtained transistors and validate the influence of all involved technological processes on the transistor parameters.

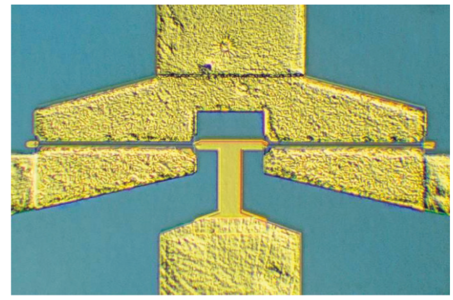

Figure 3: Construction of X-band AlGaN/GaN HEMT.

Listed previously parameters were included in the comprehensive fabrication model of AlGaN/GaN HEMT. The model was applied to the prediction of the parametric yield of saturate drain current I_{dss}. This parameter is one of the most important enabling the determination of transistor applicability into the power circuits for microwave band, specifying the maximum power that can be obtained using a single device. It is affected by a number of factors, related to AlGaN heterostructure, HEMT design, and fabrication processes parameters. The elaborated model was written in the form proposed above. The input parameters distribution was chosen on the basis of the previously analyzed results of the research on respective technological processes within the research group. In Table 1, the list of model parameters with their distributions is presented.

These parameters consist of complete input into the framework. In Figure 4, a simulation of saturate drain current, I_{dss}, and distribution for the batch of one thousand HEMTs are presented.

The figure illustrates important results for production planning regarding the values of saturate drain currents. The distribution differs from usually expected in such cases—Gaussian distribution. The simulation allows for sizes allocation of accurate quality bins.

Validation of obtained results is performed using two approaches. First, obtained results of operation parameter distributions should be consistent with measurements results that allow for analysis of prediction accuracy, as well as, further model calibration. The obtained simulation results of the distribution of saturate drain current are in accordance with measurement data from a small batch of devices fabricated during the preproduction phase at WUST. The second way to validate the model of obtained results was to perform analysis without stochastic variability. It was achieved by the reduction of involved random variables to their expected values. They are equal to the exact sizes and compositions of respective HEMT elements determined during transistor design. The distribution of three parameters that are strongly coupled with I_{dss}, 2DEG electron mobility, μ_s, AlGaN layer thickness, and 2 DEG sheet electron concentration, n_s, is presented assuming first that I_{dss} has no stochastic variability and can be determined directly. The value of I_{dss} in the form of a binary measure is

Table 1: The applied model parameters and their distributions are presented.

Parameter	Distribution type
Heterostructure sheet resistance R_s [Ω/□]	Normal (400, 10)
Heterostructure 2DEG electron concentration n_s (m^{-3})	Normal (1.15e13, 0.05e13)
AlGaN layer thickness d_{Al} (nm)	Normal (19, 1)
Ohmic contact resistance R_c (Ω)	Normal (1e-3, 2e-4)
Gate length L_g (μm)	Normal (1, 0.2)
Max carrier velocity V_s (cms^{-1})	Normal (0.75, 0.05e7)
Electron mobility μ [$cm^2V^{-1}s^1$]	Nonlinear function of R_s and ns 1/($R_s n_s$(1.6e-19))
Pinch-off voltage V_p (V)	Nonlinear function of d_{Al}, n_s
Gate source distance (μm)	Discrete (based on measurements)

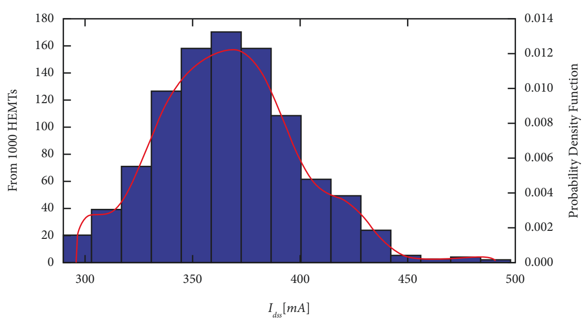

Figure 4: Distribution of I_{dss} for 1000 AlGaN/GaN HEMTs fabricated at WUST.

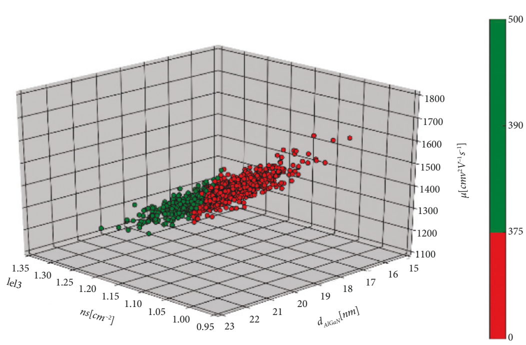

Figure 5: Relationship between saturate drain current, electron mobility, layer thickness, and electron concentration of AlGaN/GaN HEMT, when stochastic dependencies are omitted.

calculated. The threshold of I_{dss} that qualifies the HEMT as approved was set arbitrarily to 375 mA. Obtained results are presented (Figure 5).

There can be an unambiguously determined area, where approved devices can be found. In that case, for specific values of n_s, d_{AlGaN} and μ saturate drain current can be exactly calculated. Obtained values correspond to the values calculated using classical device models of HEMTs. Although measurement results clearly show that such description is incomplete and that is required to examine real statistical distributions of respective parameters. In Figure 6, the true dependence is presented in the real conditions, assuming parameters stochastic variation.

Distributions obtained with that approach correspond to the measurement results in which the range of acceptable n_s, d_{AlGaN}, and μ parameters is fuzzy. The figure clearly shows

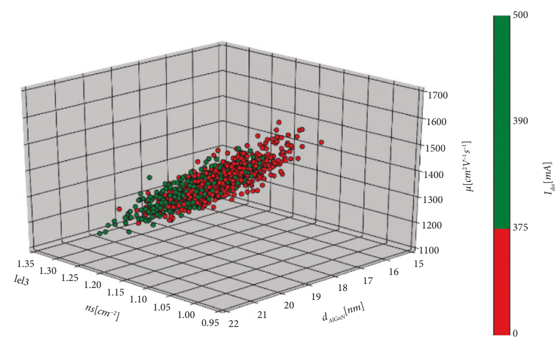

Figure 6: Relationship between saturate drain current, electron mobility, layer thickness, and electron concentration of AlGaN/GaN HEMT with stochastic complexity being considered.

the need for application of the elaborated methodology, because it allows for optimization of selected parameters with concern to the variation of the others as well as allows for the proper estimation of the parametric yield of fabricated devices.

7. Conclusions

The production process of advanced devices is of high complexity. During such process, virtually each individual technological step is under constant research and development and, as a result, requires a nonconventional approach to the question of the expected yield modelling. Described complexity results from a significant number of independent variables, available interoperation measurements, and the indeterminable influence of external factors. Dependence between the aforementioned elements is often nonlinear. The additional challenge of the conducted research is the environment of the R&D laboratory, which character limits the availability of a sufficient number of production data from various technological cycles. For the need of yield analysis, there are only available separate elements of knowledge that usually focus solely on a single technological process and relations between its input and outputs. The full picture is further shadowed by a relatively small number of experiments that hinder the statistical inference and work on the cutting-edge of the current technological capability. Despite the listed challenges, thanks to the flexibility of the developed model, there was possible to include the knowledge and experience of the research team as well as to formulate conclusions regarding the directions of optimizations to be performed. The modular structure of the simulator enables acceleration of computation by splitting them into many processing units, warranting the usability of the framework as the number of modeled relations is going to increase in the future. There is also possible to apply developed methodology into the design process of other semiconductor devices. Considering the literature reports [17–20], the application of modern methods of manufacturing processes modelling that was presented in this work can be considered as the way to drive cost reduction in the semiconductor industry as well as to create novel innovative products.

Data Availability

The source code and input model data used to support the findings of this study have been deposited in the OSF repository DOI 10.17605/OSF.IO/AVS6Q.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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