# Comparative Analysis of TCAD augmented ML Algorithms in modeling of AlGaN/GaN HEMTs

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***Abstract*— In this study, a computer-aided design (TCAD) supported machine learning framework is built to predict the intrinsic parameters of GaN HEMT, such as $V_{TH}$ (Threshold Voltage) and $g_m$ (Transconductance). TCAD was used to generate the training data set constituting the $I_D$-$V_{GS}$ characteristics of the GaN HEMT. This is achieved by changing multiple input parameters (e.g. the Al mole fraction (x), gate metal work function, AlGaN barrier thickness and gate length). We deployed numerous ML algorithms and an ANN (artificial neural network) to predict the $V_{TH}$ and $g_m$ of GaN HEMT. We compared the performance of these ML algorithms and found that the boosting and ensemble algorithms provide better results in terms of accuracy. We showed that Random Forest and Gradient Boost were most effective in predicting $V_{TH}$ with an $R^2$ value of 0.99 each, and for $g_m$ prediction, Gradient Boost was most effective with an $R^2$ of 0.92.**

***Keywords*— *ann, gan hemt, gradient boost, machine learning, tcad, threshold voltage, transconductance***

## I. Introduction

GaN HEMTs (Gallium nitride-based high electron mobility transistors) are a desirable and promising candidate for high power and high-frequency electronic applications owing to their distinct material properties such as a wide band gap (3.4 eV) and high saturation velocity ($2.5 \times 10^7 cm/s$) [1], [2]. Owing to these properties, GaN HEMTs are used for space applications [3], RADARs [4], mixers [5], THz detectors [6] and high-speed RF circuits [7]. TCAD-integrated (ML) machine learning and (DL) deep learning have gained increasing popularity in the past few years due to the availability of highly efficient computational systems [8]-[10]. Machine learning and deep learning require a large amount of data for training the models, which acts as a barrier to their usage across various industries, such as microelectronics [11]. Data generation for these HEMT devices is very cumbersome because the characterization of devices is costly and time-consuming. Therefore, it is more efficient to use TCAD for generating data by varying device structure, process, and material parameters. It is also used to establish a relationship between input and output which can further be utilized for the prediction of significant device parameters, which is otherwise a tedious process owing to the heterostructure of HEMTs and their complex device physics [12].

TCAD-augmented ML and artificial neural networks have already been used in the past to model junction-less nanowires [13], [10], and other devices [8]. However, these reported methods suffer from outliers or weak learners, leading to models not being applicable to non-linear data. Regression algorithms [14], [15] have been used in the past to predict HEMT's parameters; however, they produce inaccurate results when the relationship in the data is non-linear, non-monotonic and complex [8]–[10].

In this work, we encountered these issues using (GB) Gradient Boost [16] and (RF) Random Forest algorithms [17]. We compared the performance of different ML algorithms and determined which ML algorithm was accurate and robust for the prediction of $V_{TH}$ and $g_m$ of GaN HEMT. For the first time, we use a Gradient Boosting algorithm to predict the intrinsic parameters of GaN HEMT.

## II. Device Design, Simulation Setup and Data Set Preparations

The 2D structure of the AlGaN/GaN HEMT used in this study is illustrated in Fig. 1 (a). It has a barrier layer ($t_{AlGaN}$) of 30 nm, and the thickness of the GaN buffer ($t_{GaN}$) used is 2 µm. The drain to source spacing and gate to drain spacing is 2.5 µm, respectively. The length of the gate was 1 µm, and the width of the device was 150 µm. The transfer characteristics of the device are shown in Fig. 1 (b) [18]. The calibration [18] was done using the Sentaurus TCAD version 2018.06-SPI [19].

The TCAD Lombardi model and Philip unified mobility models are used to account for the carrier, impurity scattering and mobility degradation at the interfaces. The SRH (Shockley Read Hall) and Auger models are used for recombination properties through deep defect levels and traps. The drift-diffusion model [20] was used to set up the transport properties of carriers along with the Fermi statistics. The intrinsic device parameters investigated and varied were Al mole fraction (x), gate length ($L_G$), barrier thickness ($T_B$), and gate metal work function (WF), as shown in Table I. Fig. 2 shows a subset of the training data set used to train the machine learning model. Several Transfer characteristics ($I_D$-$V_G$) and transconducatcne curves $g_m$ of the GaN HEMT are simulated with the variation of the input parameters mentioned in Table I.

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## III. ML ALGORITHMS AND IMPLEMENTATION STRATEGY

The TCAD data generated for multiple parameters, as described in the previous section, are used in the implementation of machine learning algorithms for prediction and modelling purposes. The process flow and strategy for implementation are shown in Fig.3. Data preprocessing [21] involves importing all the libraries and cleaning the data. The data was standardized according to the z score [22] with a mean value of 0 and a standard deviation of 1, as shown in (1).

$$z = \frac{(x - \mu)}{\sigma} \tag{1}$$

After defining theinput features and output labels, the Scikit learn library [23] was used to implement the machine learning algorithms. Then, the pandas data frame [24] was used for splitting the data set into training and test set. Seventy percent of the data was allotted for training and building the models, whereas thirty percent of the data was used for evaluating the test set. Subsequently, the models were evaluated according to the coefficient of determination.

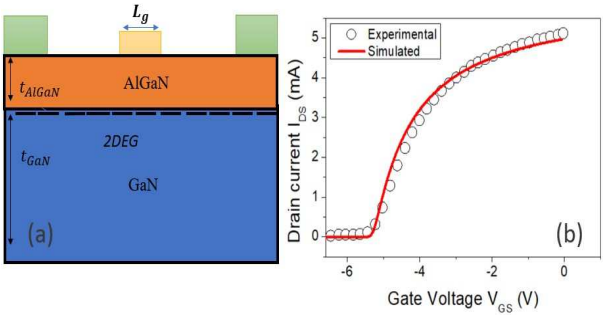


Fig. 1. a.2D device structure of GaN HEMT used for simulation b. Simulated Transfer characteristics calibrated with experimental data [18].

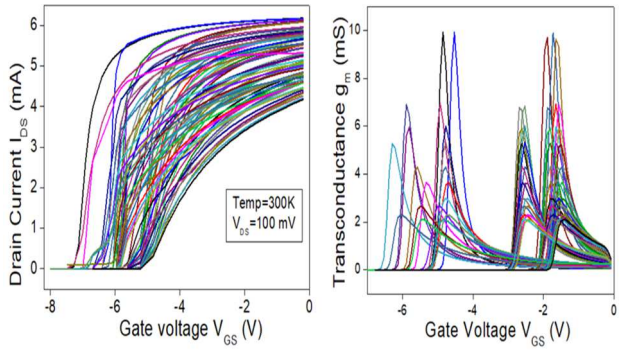


Fig. 2. Subset of Training Data a. Transfer Characteristics and b. Transconductance of GaN HEMT used for training of ML and ANN by variation of parameters in Table I.

**Table I** The list of parameters varied to create ML data set

| Parameter | Value |
|---|---|
| Al mole fraction (x) | 0.15 to 0.3 |
| AlGaN Barrier Thickness ($t_{AlGaN}$) | 18 nm to 30 nm |
| Work Function (WF) | 4.1 eV to 6.1 eV |
| Gate Length | 100 nm to 1.8 µm |

The ML algorithms used in this work for the prediction of threshold voltage and transconductance of GaN HEMT are Ridge and Lasso Regression [25], [26], Random Forest, and Gradient Boost.

## IV. RESULTS AND DISCUSSION

In this study, the first ridge and LASSO regression were used to predict the value of $V_{TH}$ and $g_m$ by varying four input parameters (Al mole fraction, AlGaN barrier thickness and gate length, and gate metal work function). Fig. 4 shows the scatter plot of the predicted and actual values of the threshold voltage and transconductance, along with the coefficient of determination $R^2$ [27]. Lasso regression gives an $R^2$ value of 0.96 for $V_{TH}$ prediction and 0.74 for $g_m$, as shown in Fig.4 (c) & 4(d). Ridge Regression gives $R^2$ value of 0.95 for $V_{TH}$ and 0.73 for $g_m$, as shown in Fig. 4 (a) and 4 (b). K-fold cross-validation was used to evaluate model accuracy after tuning the model's hyperparameters. Ridge regression provides an

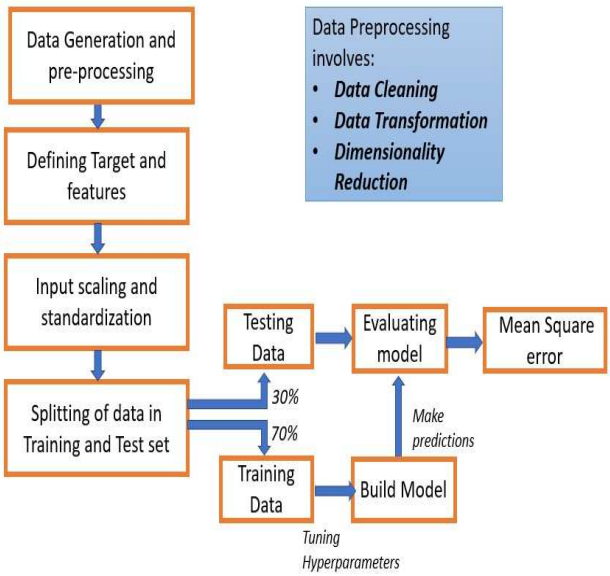


Fig. 3. Process flow diagram of Machine learning model development, prediction, and validation.

optimized mathematical equation (2) that is useful for the prediction of $V_{TH}$. The mathematical equation and their respective coefficients are given in (2) and Fig. 5, respectively.

$$V_{TH} = A(\text{Al mole fraction}) + B(\text{Gate Metal Work function}) + C(\text{AlGaN Barrier Thicnkess}) + D(\text{Gate Length}) + constant \tag{2}$$

The negative value of the coefficient (mole fraction and barrier thickness) indicates that if we increase their values, the threshold voltage will decrease and vice versa. This shows that with the decrease in mole fraction and barrier thickness, the 2DEG charge is reduced; hence, the threshold voltage is increased. An increase in work function will also increase the threshold voltage as it increases the barrier height and lifts the conduction band. This leads to fewer charges in 2DEG. [28], [29].However, ridge and lasso regression, as shown in Fig 4a-4c, were helpful in predicting $V_{TH}$. However, a lesser value of $R^2$ in the case of $g_m$ shows that these algorithms fail in the prediction when there is a non-linear, complex and non-monotonic relationship in the data. The drawback of overfitting and high bias in the regression models discussed above were solved by Random Forest and Gradient Boost

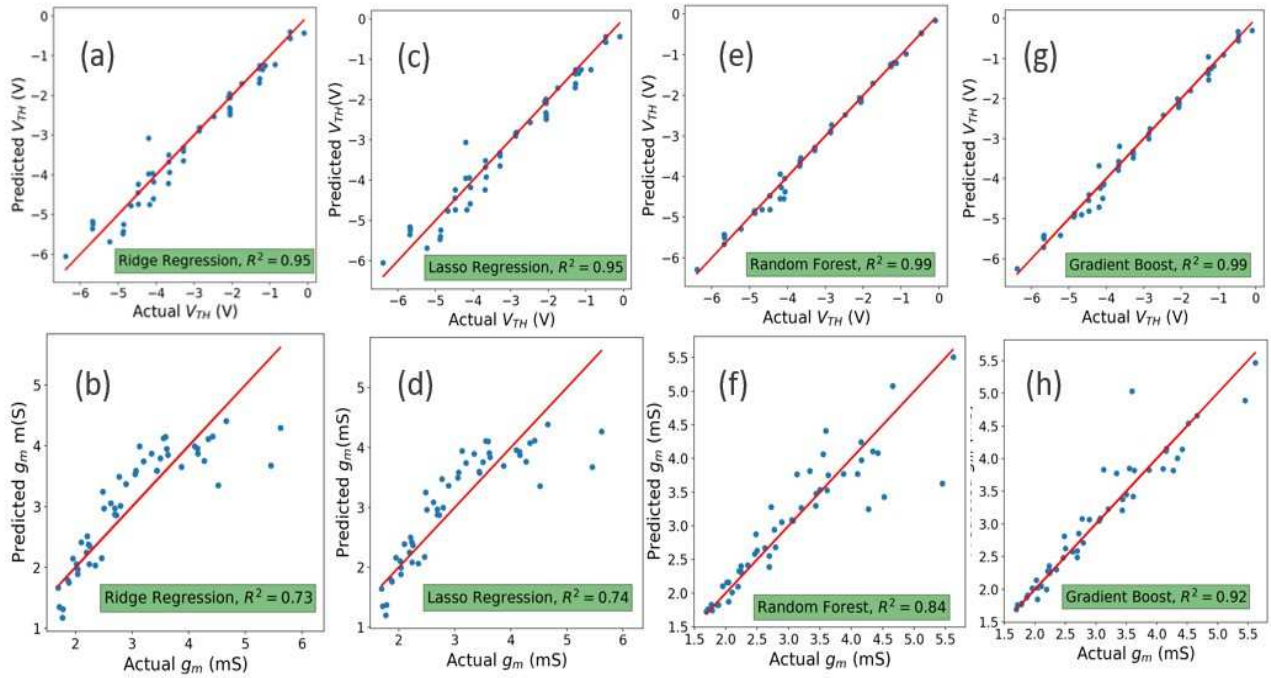


Fig. 4. Scatter plots (blue dots) along with the $R^2$ value showing the comparison of the performance different ML algorithm using test data. (a)-(b) for Ridge Regression, (c)-(d) for Lasso Regression, (e)-(f) for Random Forest and (g)-(h) for Gradient Boost.

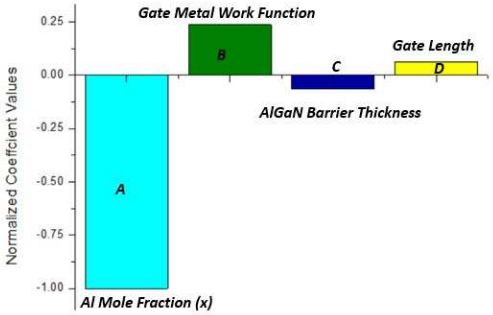


Fig. 5. Normalized Coefficients in the equation of threshold voltage developed by Ridge Regression ML algorithm.

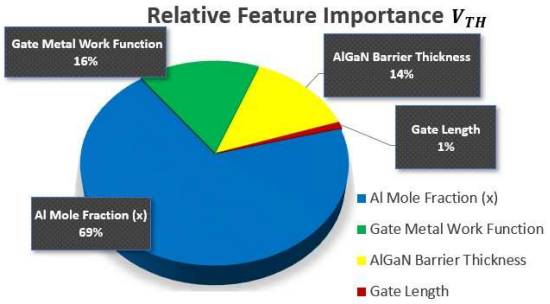


Fig. 6 Relative weight of each feature in modeling Threshold Voltage given by Random Forest ML algorithm.

algorithms. The $R^2$ value for the Random Forest for $V_{TH}$ and $g_m$ is 0.99 and 0.84, respectively, as seen in Fig. 4e and Fig. 4f, respectively. The predictions are more accurate and stable when compared to the ridge and lasso regression. This is further improved significantly by the use of ensemble and boosting algorithms, such as the Gradient Boost algorithm, which gives an $R^2$ value of 0.99 for $V_{TH}$ and 0.92 for $g_m$, as seen in Fig. 4g and Fig. 4h, respectively. This improvement is due to the fact that the Gradient Boost algorithm takes into account the non-monotonic relationship between the

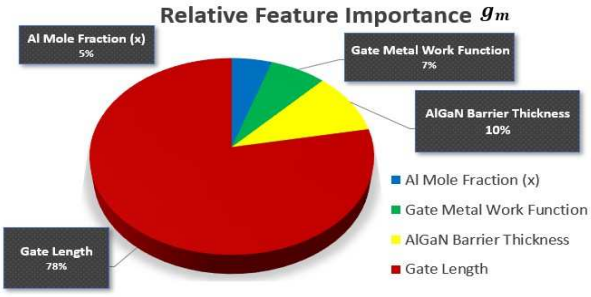


Fig. 7. Relative weight of each feature in modeling transconductance given by Random Forest ML algorithm.

variables more accurately. The weights from the random forest are shown in Fig. 6 and Fig. 7 for VTH and gm respectively. The R2 value between 0.84 to 0.99 signifies that the device physics has been captured accurately. We also developed for comparison a multi-layer Deep Artificial Neural Network is also developed for the modelling of the $V_{TH}$ and $g_m$ containing an input layer with four nodes and four hidden layers with 64, 32, 16 and 8 nodes, respectively, not shown in this work. The activation function used in the development of this ANN is the RELU [30] function, and Adam optimization [31] is used for 150 epochs.

All the results from ML model were further validated with calibrated TCAD simulations. From Fig. 8a. and Fig. 8b, it is evident that Ridge Regression is less accurate for the prediction of $V_{TH}$ and especially $g_m$, as there is a significant mismatch between the simulated and model results. The match for models of Random Forest, Gradient Boost and ANN in prediction is shown in Fig. 8(c)-(h). It can be seen that the use of Random Forest and Gradient Boost algorithm proved to be more accurate for predictions. They also have a better match, as shown in Fig 8(c)-8(h). The relative improvement in the case of $g_m$ shows how regression and regularization algorithms fail to predict when there is a non-linear relationship between input and output. A comparison

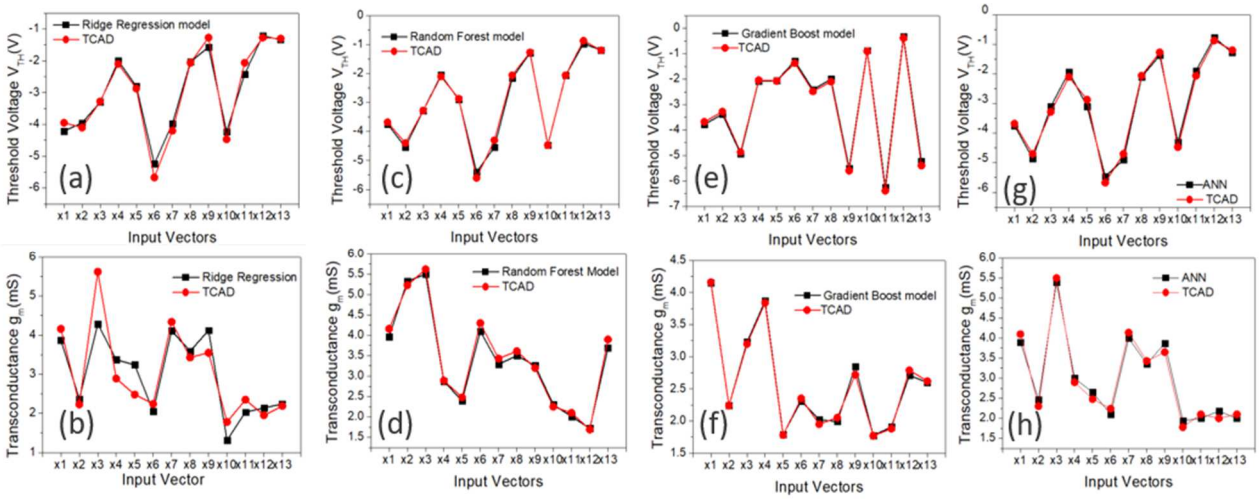


Fig. 8. Comparison of model results and TCAD results for (a) and (b) Ridge regression , (c) and (d) Random Forest , (e) and (f) Gradient Boost, (g) and (h) ANN .

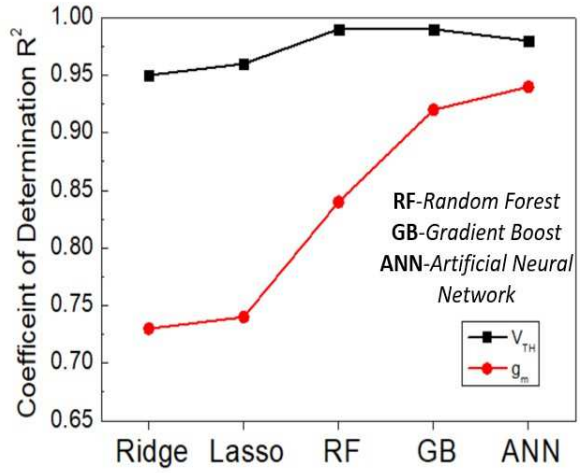


Fig. 9. Comparison of the different ML algorithms and ANN in the prediction of $V_{TH}$ (black dots) and $g_m$ (red dots), respectively.

of all the algorithms related to their prediction of $V_{TH}$ and $g_m$ was performed using the coefficient of determination, as shown in Fig. 9. The better results of Random Forest are due to the fact that it averages out results from all the trees and provides the output. The Gradient Boost algorithm ensures boosting the performance of weak learners among the data and hence improving results. These ensemble and boosting algorithms provide performance at par with ANN, which is a good thing as implementation requires ANN to have more GPU power, is slower and requires more data. [32]

## V. Conclusion

Ensemble and boost algorithms (i.e., Gradient Boost algorithm) and Random Forest algorithm are used to predict $V_{TH}$ and $g_m$ based on structural and material parameters. Ridge and Lasso regression were also implemented to develop a mathematical equation that helps in modelling $V_{TH}$. It was found that regression algorithms were not efficient in the prediction of $g_m$ with an $R^2$ value of 0.73. Hence, the Random Forest and Gradient Boost ML algorithms, which are a collection of decision tree models, were implemented, which improved the prediction of $g_m$ with an $R^2$ value of 0.84 and 0.92, respectively. Furthermore, the performance of the Gradient Boost algorithm was found to be at par with that of ANN.

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