Accuracy of Machine Learning Models on Predicting the Properties of Vertical GaN Diodes

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Abstract

Manufacturing of vertical GaN devices is important to its future use in high power electronics. However, the current process is not mature, resulting in non-ideal behavior. To improve manufacturing of GaN, reliable screening techniques are essential. Machine Learning has proven useful for quality control in several fields though its use on wide bandgap semiconductors is limited. This paper discusses several Machine Learning models used with optical profilometry to predict the quality of GaN diodes and their accuracy.

I. Introduction

GaN wafer manufacturing and epitaxial growth have improved in recent years making vertical GaN technology a candidate for next generation high-power electronics[1]–[3]. To meet the industry standard, wafer screening techniques such as photoluminescence, Raman spectroscopy, x-ray tomography, optical profilometry, and cathodoluminescence have been proposed [4]. It is well established that these techniques can detect defects that cause failures. However, the analysis is not always straightforward. Therefore, novel analysis techniques such are Machine Learning are useful to explore.

Machine learning has proven useful for the semiconductor industry. Positive results have been obtained from computationally-generated data from TCAD modelling [5]–[8]. However, experimental reports are limited. This is likely due to the large number of datapoints required for training the models.

It is likely that the ideal algorithm will involve a combination of several techniques. However, with machine learning it is useful to determine which techniques correlate with each desired output characteristic since adding unimportant variables to the model can reduce its accuracy. This paper focuses on using optical profilometry to predict the forward and reverse bias behaviour of diodes. That measurement is useful for investigating substrate quality since it is sensitive to many different types of defects. However, it can be difficult to detect whether a specific section of the wafer is suitable for device growth by quick observation. This is because the bumps, pits, and rough patches require complicated analysis to detect. Several measurements can be used to identify these rough patches including the rms roughness, the number of outlier points (bumps and pits), and the height/depth of the defects. This talk focuses on the effectiveness of machine learning models at predicting forward and reverse bias conditions - including low voltage leakage current, ideality factor, turn-on voltage, and turn-on resistance - using optical profilometry data.

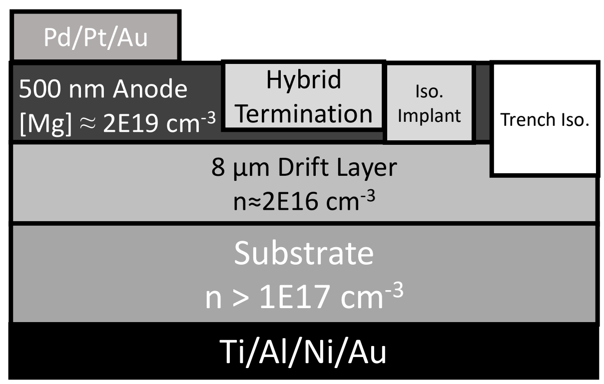

Fig. 1. (Side View) Diagram of vertical GaN diodes used in this study.

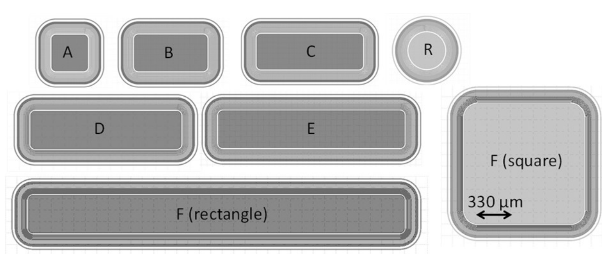

Fig. 2. A top view, to scale image of all the diode sizes used in this study with appropriate labels. Device areas range from (10^{-3} - 10^{-2} cm^2).

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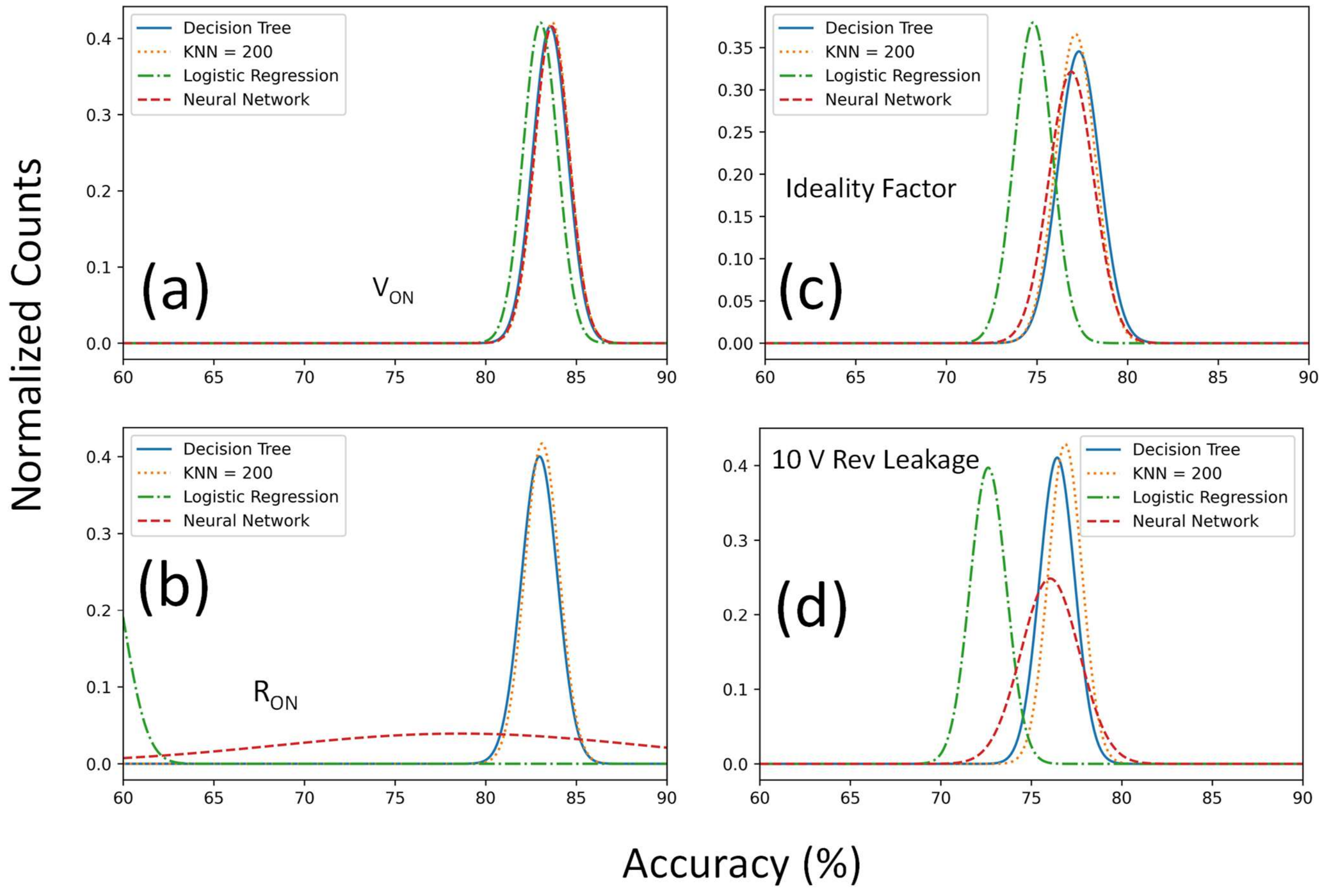

Fig. 3. The accuracy distribution of the models at predicting the pass rate of the turn on voltage (a), on-resistance (b), ideality factor (c), and 10 V reverse leakage (d). Distribution was determined by constructing a gaussian from 100 results.

II. Experimental

A. Sample Fabrication

Vertical P-i-N diodes (Fig. 1) were processed using methods from our previous work [9]–[11]. Our team at Sandia National Laboratories grew in situ two GaN layers using the Taiyo Nippon Sanso MOCVD SR4000HT reactor and 10 different GaN substrates. An 8 μm drift layer, doped with Si at n ≈ 2×10^{16} cm^{-3} and a subsequent p-layer approximately 500 nm thick were grown. The p-layer was doped with [Mg] ≈ 2×10^{19} cm^{-3} giving an estimated hole concentration p ≈ 5×10^{16} cm^{-3} at room temperature. Vertical diodes were fabricated with many shapes and sizes (see Fig. 2). The diode fabrication included a backside Ti/Al/Ni/Au layer and a topside Pd/Pt/Au layer. A trench isolation layer was etched outside the devices using an Ar/Cl2 plasma and a ~ 600 nm multi-energy nitrogen implant with a box profile was done for further isolation within the trench. The diodes also included an implanted guard ring/JTE hybrid termination

B. Optical Profilometry Data Collection (Input Data)

Before device fabrication, optical profilometry measurements were taken on 2-inch vertical GaN PiN junctions with an x-y resolution of 4421 nm/pixel and a sub nanometer z axis resolution as described in our previous research [12]. All measurements were taken with the Zygo™ NewView 7300 optical profilometer.

After the measurements, the data were divided into small regions 325 x 325 μm in size. In each region, the RMS roughness was calculated as

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(Z_i - Z_{avg}\right)^2})$$

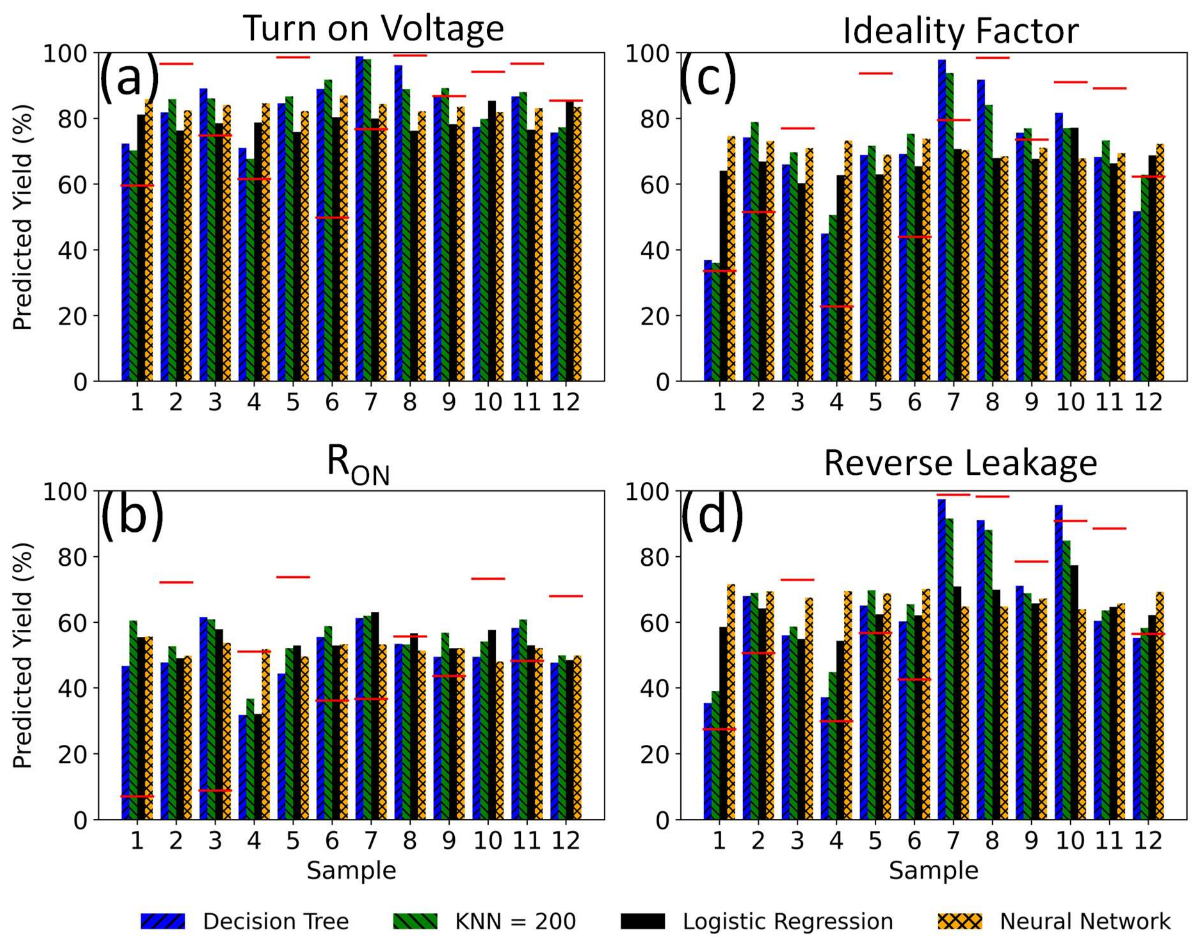

Fig. 4. The accuracy of the four machine learning models at predicting each variable- (a) Turn on Voltage (b) On Resistance (c) Ideality Factor and (d) Reverse Leakage at 10V- is shown. The models were trained on all the wafers except the one being tested in all cases. The red line represents the experimental result.

where Z is the height of each region, and the area of bumps and pits was calculated using an extreme Studentized deviate test for outliers as described in previous research [13]–[15].

C. Electrical Data Collection (Output Data)

The data was collected using a custom built auto probing system and several electrical instruments. Forward bias and low voltage reverse bias (10 V) measurements were taken using a Keithley 4200 Source Meter Unit (SMU) with a preamplifier and 10 atto-amp measurement resolution. The measurements were taken on twelve wafers.

D. Machine Learning Models

Four simple machine learning models from the Sklearn Python package were used to determine pass/fail for each device. Those models were decision Tree, K-Nearest Neighbor (k=200), Logistic Regression, and a two-layer Neural Network with a logistic activation function. These models are discussed in more detail in other works. Since the number of devices is of the order of thousands, not millions, a binary pass-fail value is a more reliable metric. All models were trained to predict three different behaviors with pass criteria listed:

a. turn on voltage 2.8-4.8 V
b. on-resistance < 10 mΩ-cm^2
c. ideality factor < 2.5
d. 10 V reverse bias leakage < 100 nA

The accuracy of all the variables was calculated by randomly sorting 80% of the data into a training section, and 20% into the test section. The models were constructed using the trained data and their accuracies were tested using the test data. This test was repeated 100 times for each model testing each variable individually. The accuracy of the tests is shown in Fig. 3.

III. DISCUSSION

From the results in Fig. 3, all models have similar accuracies in most cases. The models work especially well for Low Voltage Leakage and ideality factor with all being consistently over 75% accurate. When predicting turn on voltage and R_{on} passage, the neural network and logistic regression methods often made inaccurate predictions. For high voltage predictions, the neural network failed to converge.

To test the accuracy of these methods at predicting the device yields on the wafer, all models were trained on all wafers excluding one, and tested on the remaining wafer. The results (shown in Fig. 4) reveal that this method is effective in most cases. When testing V_{ON} the prediction accuracy is good, but the experimental pass rate of all the devices is quite high, this causes the model while training to put all borderline devices in the pass category, which could artificially raise the accuracy. The R_{ON} is also shown to be difficult to predict with optical profilometry. Though with many of the wafers in Fig. 4b, the models do predict the experimental result accurately, the individual devices results for two of the models in Fig. 3b result sometimes produce low accuracy. Additionally, the neural network model often failings to converge thus predicting passage rates of 0% or 100%, giving a wide distribution of accuracies in Fig. 3b though it is possible to train a neural network with similar accuracy to other models as done in Fig. 4b though it takes several iterations. The ideality factor and reverse leakage current passage rates appear to be well correlated thus the experimental and predicted passage rates are similar as seen in Fig. 4c-d. Additionally, all four models produce similar accuracy distributions as show in Fig. 4c-d indicating that these variables correlate with optical profilometry results well.

Though all the models are reasonable at predicting results, decision tree stands out as particularly useful because it is the simplest to train, the computers decision making process can be directly seen, and it is less affected by adding unimportant variable to the models, thus this model produces high accuracy for all four variables. The most important variable for V_{ON} was the RMS roughness, for R_{ON} the device size, and for the Ideality Factor and Reverse Leakage the area of bumps and pits near the device.

IV. CONCLUSIONS

In summary, optical profilometry measurements were combined with machine learning to produce models capable of pass-fail predictions for vertical PiN diodes. It was determined that Ideality Factor and Low Voltage Leakage are well predicted using optical profilometry, while R_{ON} and V_{ON} had inconclusive results. The passage rate was too high with V_{ON} to make a definitive answer, and the R_{ON} had an inconsistent accuracy. Likely the R_{ON} depends more on the fabrication process than on the pre-existing conditions of the wafer. However, the high accuracy of the Decision Tree and KNN=200 models show there is potential to predict this quantity using machine learning with optical profilometry. Predicting the exact values of these variables with these methods would require more data and a more complex model such as a convolutional neural network on the optical profilometry data.

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Acronyms

R_{ON}: On Resistance
V_{ON}: Turn on Voltage
JTE: Junction Termination Extension
Rev: Reverse