Development of compact Schottky diode model on GaN

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Abstract. In the article the technique of formation of compact (SPICE) model of Schottky diode on GaN, manufactured by heteroepitaxial growth on a sapphire substrate (Al₂O₃) is considered. As a compact model, the modified model of a conventional diode on the p-n junction is used. The procedure is proposed for extraction of Spice parameters of the Schottky diode model on the basis of experimental volt-ampere (VAC) and volt-farad characteristics (VFC) using the Matlab computer mathematics system. The procedure for extracting the parameters of the compact model and the electrophysical characteristics of the device can be useful for commissioning the technological process for Schottky power diodes production.

1. Introduction

A compact model is a virtual analog of a real device. The purpose of the compact model [1] is to provide users with reference material on the parameters of the manufactured instrument.

In addition, this model is used at the stage of the circuit design of microelectronic devices, including integrated circuits.

The synthesis of the compact Schottky diode model can be carried out in two ways:

1. On the basis of the theoretical calculation of the complete model (VAC and VFC) by numerical solution of the system of fundamental equations (in the diffusion-drift and / or hydrodynamic approximation) with the help of one of the programs of device-technological modeling (for example, Sentaurus TCAD) with subsequent extraction the parameters of compact model from it.

2. By extracting the parameters of the compact model from the experimental data: VAC, VFC, and temperature dependences of the Schottky diode current.

The first approach gives satisfactory results only for silicon technology, which provides rather high accuracy of simulation due to the presence of a large number of perfect models of electrophysical parameters.

In the case of fabrication of devices on complex semiconductors, the second approach based on experimental data is more effective.

An additional advantage of this approach is the possibility of extraction of a number of electrophysical parameters: the height of the Schottky barrier, the concentration of impurities in the substrate, the density of surface states at the metal-semiconductor interface, the Richardson constant.

Although these parameters are not parameters of the compact model, nevertheless, they are extremely important from the point of view of evaluating the quality of the diode manufacturing process.
2. Compact (SPICE) Schottky diode model
The compact model (Figure 1) includes a set of parameters used to simulate the device in different modes of operation: static (DC), dynamic (for transient analysis, TR) and frequency-response (in small signal mode, AC).
Each of the listed modes of analysis has its own set of parameters.

![Figure 1. Full equivalent circuit of Schottky diode.](image)

In most SPICE-like programs for circuit simulation, the compact (SPICE) Schottky diode model is a variation of the conventional diode model on p-n junction. The main difference between them is that the equivalent circuit of the Schottky diode (Figure 1) does not contain the diffusion capacitance, which is responsible for the processes of accumulation and discharge of minority charge carriers. Therefore, for the transition from conventional diode model to Schottky diode model it is sufficient to equate to zero the transit time of charge carriers of the diode base. In the SPICE model, this time corresponds to parameter $\text{TT} = 0$, used to simulate the diffusion capacity.

In this article, in order to obtain the compact Schottky diode model, three types of parameters were extracted, used for:
- simulation of static operation mode in direct switching: $I_s$, $n$ and $R_s$. These parameters are extracted from the experimental results of measuring the direct branch of VAC;
- simulation of static operation in reverse mode: $R_p$, $BV$ and $IBV$. These parameters are extracted from the experimental results of measuring the reverse branch of VAC;
- simulation of the dynamic (transient) mode of operation in the process of switching, for example, from one static mode to another. This process is related to the presence of a parasitic barrier capacitance $C_d$ in Schottky diode, which is modeled by a set of corresponding parameters ($C_{JO}$, $V_J$, $M$), for extraction of which the results of measurements of diode VFC are used.

3. The method of extraction of parameters of compact model
Two types of numerical analysis methods were used to extract the parameters of the compact Schottky diode model from experimental data [2]: polynomial approximation (polyfit) by the method of least squares (OLS) and the technique based on the mathematical apparatus of optimization theory. Both of these tools are included in the tool kit of the Curve Fitting ToolBox of the computer mathematics system MATLAB.

3.1. Extraction of static parameters
To extract the static parameters of Schottky diode, simplified version (Figure 2) of the above mentioned equivalent diode circuit is used-without the barrier capacitance $C_d$.

3.1.1 VAC of diode in direct switching. For the diode forward-bias region of VAC, the parallel leakage resistance can be neglected, which corresponds to the equivalent circuit shown in Figure 2.
This equivalent circuit corresponds to the mathematical expression:
\[ i = I_s \times \exp((v - i \times R_s)/(n \times \phi_p)) - 1 \],
which includes three parameters:
- \( I_s \) – saturation current (\( I_S \) in compact model);
- \( n \) – coefficient of non-ideality (\( N \) in compact model);
- \( R_s \) – resistance of the base region (quasi-neutral region of diode). It corresponds to \( R_S \) in compact model.

In the case where the input voltage exceeds 0.1 V, expression (1) can be simplified, resulting in the form:
\[ i = I_s \times \exp((v - i \times R_s)/(n \times \phi_p))). \]

This is a transcendental equation, which can only be solved by a numerical method.

To estimate the values of the static parameters of the diode (\( I_s, R_s \) and \( n \)), they must be extracted from the experimental data (the direct branch of VAC of the diode). In numerical mathematics, this procedure is called the approximation of tabular data with the help of appropriate analytic function with a set of necessary parameters. In our case, this is the exponential function (2) with parameters \( I_s, R_s \) and \( n \).

To extract the static parameters of the Schottky diode, we used an experimentally-removed VAC in the direct switching (Figure 3).

Due to the complexity of the task, the extraction procedure for three parameters was performed in two stages:
1. In the region of low voltages 0.1-0.3 V, the resistance \( R_s \) can be neglected. As follows from the published data and is confirmed by the experimental data shown in Figure 4, the thermionic charge transfer mechanism dominates in this section of VAC. This allows us to use it to estimate the values of parameters \( I_s \) and \( n \).
2. Then, using expression (2) and the obtained values of the two parameters, the third parameter, the quasineutral resistance $R_s$, is estimated for the entire range of currents and voltages of the direct branch of VAC.

**Extraction of $I_s$ and $n$ parameters.** In the region of small values of forward-bias (in the range of 0.1-0.3 V), the influence of the series resistance $R_s$ can be neglected, which makes it possible to convert expression (2) to the form:

$$i = I_s \cdot \exp(v/(n \cdot \varphi_T)).$$

(3)

To simplify the procedure of extracting $I_s$ and $n$ parameters included into this expression, the original expression should be logarithmized, transforming to the form:

$$\ln(i) = v/(n \cdot \varphi_T) + \ln(I_s).$$

(4)

The resulting expression describes a straight line in coordinates $v$ and $\ln(I_s)$ with a slope $1/(n \cdot \varphi_T)$ and the point of intersection with the coordinate $y$ corresponding to the saturation current $I_s$. Thus, the static parameters of diode $n$ and $I_s$ can be extracted from the experimental data after the approximation of the latter by expression (4).

In MATLAB program for the approximation of experimental data, the straight line provides the `polyfit` function that finds the coefficients of the polynomial $P(x)$ of $n$ degree. The general expression for this function is:

$$coeff_{xy} = polyfit(x, y, n),$$

(5)

where $x$ and $y$ are the vectors of the values of the argument and the functions in the columns of the table (in our case they correspond to the voltage vectors ($v$) and current ($i$)).

$n$ is the degree of the polynomial used to approximate the table data.

In our case, to approximate a straight line, we must specify a polynomial of the first degree ($n = 1$) containing two coefficients $c_0$ and $c_1$:

$$coeff_{xy} = c_0 + c_1 \cdot x.$$  

(6)

Comparison of expressions (4) and (5), indicates that $c_0 = \ln(I_s)$ and $c_1 = 1/(n \cdot \varphi_T)$.

After estimating the values of coefficients $c_0$ and $c_1$ using expression (5), we determine the values of two required parameters $I_s = 8.2153e-9$ and $n = 1.2509$.

The curve shown in Figure 4 indicates a good agreement of the experimental data with the results of modeling of VAC at the initial section.

![Figure 4](image-url)

**Figure 4.** Fragment of the initial section of the experimental VAC (red circles) and the model (solid) obtained from formula (4) for two values of the extracted parameters: $I_s = 8.2153e-9$, $n = 1.2509$. 
**Estimation of the height of Schottky barrier.** Since the value of the coefficient of coefficient nonideality is different from one, it can be concluded that in this section of VAC there is a combined mechanism for transfer of charge carriers with the dominance of the thermionic mechanism [3]. The latter allows us to make an approximate estimate of the Schottky barrier height (for accurate estimate, it is necessary that \( n = 1 \)).

\[
I_s = (A \cdot R \cdot T^2) \cdot \exp(-\phi_{bo}/\varphi_T) \tag{7}
\]

Solving this equation with respect to the height of Schottky barrier \( \phi_{bo} \), we obtain: \( \phi_{bo} = 0.6957 \) V

Analyzing the result obtained, it is worth noting that the estimated value of the barrier is understated, in fact representing the value of the effective Schottky barrier. This is due to the fact that the value of non-ideality coefficient is different from one, which is characteristic of ideal Schottky diode, which indicates the combined carrier transfer mechanism. This is most likely a variant of thermionic-field emission (Thermionic-field emission, TFE), as a result of which electrons with thermal energy of less than Schottky barrier height can tunnel through the depletion region at the interface.

**Extraction of the resistance of the quasineutral region of diode \( R_s \).** As already noted, the real Schottky diode, in addition to the space-charge region, also contains a quasineutral region, which, in combination with the contact resistance, is modeled by the resistance \( R_s \) (see Figure 2).

This resistance begins to affect the characteristics of the diode in the region of increased current values, reducing the effective voltage loss across the space charge region of Schottky diode by amount \( i \cdot R_s \).

Here, for extraction from experimental data of parameter \( R_s \), we use the functions \( \text{fittype} \) and \( \text{fit} \), which are part of the tool kit of the MATLAB computer mathematic system Curve Fitting ToolBox. The first of the mentioned functions forms the objective function, the second starts the process of extraction of the required parameters.

**Formation of the objective function.** At the first stage, it is necessary to specify the objective function, which is the expression used to approximate the experimental VAC. In this case, as the objective function, we use expression (2), solved with respect to the voltage on the diode \( v \):

\[
v = i \cdot R_s + n \cdot \varphi_T \cdot \ln(i/I_s) \tag{8}
\]

After substituting in it the values of the parameters extracted at the previous stage \( I_s = 8.2153e-9 \) and \( n = 1.2509 \), and also the value of the thermal potential \( \varphi_T = 0.0259 \) V we obtain the final expression for the objective function:

\[
v = i \cdot R_s + 0.0324 \cdot \ln(i/8.2153e-9). \tag{9}
\]

We form the objective function using expression:

\[
f_{\text{type}} = f_{\text{fittype}}('x \cdot R_s + 0.0324 \cdot \ln(x/8.2153e-9)').
\]

Here, \( x \) is the vector of current values of VAC.

Then we start the procedure for extracting the parameter \( R_s \) using operators \( \text{fresult} \) and \( \text{fit} \):

\[
f_{\text{result}} = \text{fit}(x,v,f_{\text{type}},'\text{StartPoint}',[8]) .
\]

Here, \( x \) and \( v \) are current and voltage vectors of experimental VAC;

\( f_{\text{type}} \) - expression of the objective function (9);

\( \text{StartPoint} \) - initial approximation of the desired parameter, from which the search for unknown parameter begins (in this case, the value of \( R_s^{(0)} = 8 \) \( \Omega \) is set).

As a result of the calculation, we get parameter value \( R_s = 9.173 \).

Thus, the equation used to approximate the direct branch of VAC takes form:

\[
v = i \cdot 9.173 + 0.0324 \cdot \ln(i/8.2153e-9) \tag{10}
\]

Below in Figure 5, a comparison of the experimental VAC with that described by expression (10) is given. It can be seen that the greatest difference for the two curves is observed in the voltage range 0.5-1.5 V. This is due to the fact that in this range the value of the non-ideality coefficient is a function
of the applied voltage (Figure 6), which is associated with an increase in the role of the field transfer mechanism carriers (tunneling) with increasing voltage.

Figure 5. VAC of Schottky diode in direct switching: points - experiment; The solid line is the compact model ($I_S = 8.2153e - 9$, $N = 1.2509RS = 9.173$).

In the framework of the built-in SPICE model of diode a more accurate simulation of the experimental curve is almost impossible due to the use of only one averaged value of non-ideality coefficient. Therefore, in order to obtain more accurate model, it is necessary to develop a special macromodel of diode that takes into account various mechanisms of charge carrier transfer.

Figure 6. Dependence of non-ideality coefficient $n$ on the voltage.

Note. Function (10) represents a nonlinear equation. Therefore, in order to construct a model VAC on the basis of this model, a multiple solution of the given equation for various voltage values is necessary. In MATLAB program, solve() function is provided for this purpose.

To solve this problem, this function is represented as:
solve('f(x)', x)

where:

'f(x)' is the solvable equation (in this case (10)) written in single quotes;

x is the sought unknown value.

Below is an example of the implementation of this procedure when solving equation (10) for the voltage value v = 0.5 V:

\[
\text{solve('x * 8.043 + 2.622 * 0.0259 * log(x/2.794e - 7) - 0.5 = 0', x),}
\]

the start of which allows one to estimate the value of the current flowing through the diode:

\[x = 0.41904029609134856432949733350643e - 3.\]

Defining additional parameters. In addition to extracting SPICE parameters of Schottky diode model from the direct branch of VAC, two additional parameters can also be estimated: the voltage drop for the direct-on-turn \(V_{np}\) and the current density at which the self-heating of the diode begins, \(J_h\). For the estimation of both parameters, the above VAC (see Figure 3) is presented in new coordinates (Figure 7): current density-voltage [4]. From this curve, we can estimate the value of \(V_{np} \approx 2.4B\) (for the current density of 100A/cm\(^2\)). The second parameter is that the current density \(J_h\) should have a value of \(\sim 103A/cm^2\). For considered diode, the maximum current density is 312.5A/cm\(^2\), which is much lower than current density at which diode self-heating occurs. The latter is most likely due to the large magnitude of the series resistance limiting the magnitude of the current flowing through diode.

Figure 7. Dependence of the current density on the voltage for the direct branch of VAC.

3.1.2. VAC of the diode in reverse switching. For the reverse branch of VAC, the dominant contribution in VAC introduces the leakage resistance (at least in the initial stage), so the equivalent circuit will take the form shown in Figure 8.
In the region of small reverse voltages, this scheme corresponds to the mathematical expression:

$$i = \frac{v}{R_p},$$

(11)

which includes one parameter: $R_p$ - leakage resistance.

As in the previous case, we will use VAC to extract this parameter (Figure 9).

Analysis of VAC indicates that, in the voltage range $[0, 4 \text{ V}]$, the diode is shunted by the leakage resistance, as evidenced by Figure 10, where a fragment of the initial section of the reverse VAC with a higher resolution is shown (in 0.1 V increments).
In this section of the BAX, the reverse diode saturation current is masked by the leakage current, the components of which are surface leakage currents and leakage currents of dislocation nature. As noted, in SPICE, to simulate the presence of leakage current in an equivalent diode circuit, leakage resistance $R_p$ is introduced.

To estimate the magnitude of this resistance, let us perform approximation of the initial portion of the VAC by straight line. As with the extraction of $I_s$ and $n$ parameters for the direct branch of VAC, we use the polynomial function \texttt{polyfit}, which approximates experimental data by a polynomial of the first degree (6).

After setting the values of the voltage vectors $\langle v \rangle$ and current $\langle x \rangle$, we start the procedure of extraction of two coefficients of the polynomial

\[ p_{1\_fit} = \text{polyfit}(v,x,1) \]

As a result of the calculation we obtain \( c_1 = 0.4169e-8 \), \( c_0 = 0.366e-8 \). So far as \( c_1 = 1/R_p \), we find \( R_p = 1/c_1 = 2.4e8 \Omega \).

Comparison of the experimental data with the results of the calculation is shown in Figure 10.

\textbf{Estimation of the breakdown voltage.} Analyzing the behavior of the reverse branch of VAC for voltages exceeding 4V, one can see (Figure 9) that change in the voltage within two orders of magnitude ($\sim$ 95V) leads to increase in current by four orders of magnitude. This indicates a nonlinear dependence of the current on the voltage, which may be due to the action of complex of causes, including thermionic current, generation-recombination current of depleted region, and thermal-field (tunnel) current. Identifying the role of each of these components is the independent task that requires additional research. Nevertheless, from a formal point of view, the presence of this section on the reverse branch of VAC can be modeled by introducing an additional nonlinear resistance into the equivalent circuit, which would require abandoning the standard diode model and switching to the synthesis of its macromodel.

One of the main parameters of diodes intended for power electronics is breakdown voltage $V_B$, which in compact model is associated with two parameters: actual breakdown voltage $V_B$ and $IBV$ current at which breakdown is observed. As in the case of the earlier estimate of the voltage loss for the direct displacement $V_{pr}$, it is also necessary to present inverse branch of VAC given in Figure 9 in new coordinates: current density-voltage.

When analyzing the results shown in Figure 11, we use the criterion for estimating breakdown voltage value proposed in [5]. It corresponds to current density of 10 A/cm². As a result, we get

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure10.png}
\caption{Fragment of the initial section of the reverse branch of the VAC (points) and its approximation with leakage resistance $R_p=2.4e8 \Omega$ (solid line).}
\end{figure}
It should be noted, that the obtained value of breakdown voltage does not reach the theoretical values predicted at 700V, which is most likely due to the imperfection of the heteroepitaxy of gallium nitride due to the presence of high dislocation density.

**Figure 11.** Dependence of current density on voltage for the reverse branch of VAC.

### 3.2. Extraction of dynamic parameters

To design circuits using Schottky diodes in the transient mode or for frequency-response analysis, an equivalent diode circuit (see Figure 1) should contain parasitic barrier capacitance $C_d$. For the diode based on p-n junction, the SPICE capacitance model is approximated by expression:

$$
C_d = C_{JO} \ast \left(1 - \frac{V_{di}}{V_J}\right)^{-M}, \tag{12}
$$

where

- $V_{di}$ is the voltage loss on the space charge region of Schottky diode (since the barrier capacitance is measured at reverse bias, this is actually the voltage $v$ applied to the diode);
- $C_{JO}$ is the barrier capacitance at zero bias at the p-n junction;
- $V_J$ is the value of the contact potential difference;
- $M$ is the coefficient that depends on the type of impurity distribution profile in the region of p-n junction.

In the case of Schottky diode, parameter $V_J$ is understood as the barrier height at the semiconductor-metal interface. Usually for it the coefficient $M = 0.5$, which is analogous to the case of sharp p-n-junction with constant impurity concentration in the base region. Therefore, for ideal Schottky diode, formula (12) takes form:

$$
C_d = C_{JO} \ast \left(1 - \frac{V_{di}}{V_J}\right)^{-0.5}, \tag{13}
$$

To extract the SPICE parameters of the barrier capacitance, we use experimental VFC (see Figure 14).

Before proceeding with the procedure of extracting the barrier capacitance parameters, it is necessary to determine the expression for calculating the barrier capacitance. As already noted, this can be either (12) or (13). The criterion of choice can be the form of the VFC, constructed in coordinates, the graph of which is shown in Figure 12.
For a sharp jump p-n-junction \( M = 0.5 \), this graph is a straight line. In our case, there are two linear sections on the graph, which indicates the presence of two regions with different levels of doping \[6\]. Therefore, as the approximating function, we use expression (12).

![Graph](image.png)

**Figure 12.** The graph of dependence \( 1 / C^2 = f(v) \).

As in the case of parameter \( R_s \) extraction, we use the set of functions \( \text{fittype} \) and \( \text{fit} \) to extract the parameters of the barrier capacitance \( [CJO/VJ] \) and \( M \).

First, we define objective function using expression (9):

\[
ftype = \text{fittype}('CJO/(1 + x/VJ)^M'),
\]

where in quotes approximating function is specified, \( x \) is the voltage vector.

Note. We note that in the last expression, in comparison with expression (12), the minus sign is replaced by a plus sign. This allows you to enter positive values for reverse bias.

Further, to extract these parameters, we use function \( \text{fit} \), which in this case has form:

\[
fresult = \text{fit}(x, cr, ftype, 'StartPoint', [CJO/VJ M]).
\]

where
- \( x \) is the voltage vector (table voltage values);
- \( cr \) is the vector of barrier capacitance values (tabular values of barrier capacitance);
- \( ftype \) is approximating function with extracted parameters;
- \( \text{StartPoint} \) is the operator used to specify the initial values of extracted parameters;
- \( [CJO/VJ M] \) is the vector of initial values of extracted parameters.

Substituting in (11) the values of the components of the vector of initial values, we obtain:

\[
fresult = \text{fit}(x, cr, ftype, 'StartPoint', [7.5, 1.0, 0.5]).
\]

Starting the calculation, we get the estimate of the extracted parameters:

\[
CJO = 7.484 \times 10^2 (7.438, 7.53);
VJ = 1.027 (0.9672, 1.087);
M = 0.3194 (0.3138, 0.3251),
\]
where the values of confidence intervals at 95% for each of the extracted parameters are indicated in parentheses.

As a result, we obtain an expression approximating the experimental VFC:

\[ C_{\text{mod}} = \frac{7.484}{(1 + x/1.027)^{0.3251}}. \]  

(15)

Comparison of the experimental and calculated VFC shown in Fig. 13, indicates a good agreement between calculation and experiment.

![Figure 13](image)

**Figure 13.** Comparison of VFC: experimental (circles) and model (solid line), calculated by formula (15).

### 4. Conclusion

In this work, extraction from experimental data of nine SPICE parameters of Schottky diode model on GaN was performed. Eight of them (\( IS, n, RS, BV, IBV, CJO, VJ \) and \( M \)) are directly represented in the compact Schottky diode model described by the listing below:

Model DSGAN D 
\[
\begin{align*}
IS &= 8.215 \times 10^{-9} \\
n &= 1.2509 \\
RS &= 9.173 \\
BV &= 97.5 \\
IBV &= 1.96 \times 10^{-4} + \\
CJO &= 7.484 \\
VJ &= 1.027 \\
M &= 0.3194
\end{align*}
\]

The ninth parameter \( RP \) (leakage resistance) is not included directly in the list of parameters of compact Schottky diode model (see Figure 14). It is used as tuning parameter that replaces the default value of the similar parameter in SPICE diode model.

Due to the fact that the characteristics of a real Schottky diode on gallium nitride are quite different from the characteristics of ideal diode, the diode model built into the SPICE program requires perfection. This can be done by synthesizing the original model, implemented as a macromodel. However, at this stage of the development of production technology of such diodes, this is hardly advisable because of imperfect production technology itself. Nevertheless, the method of extraction of parameters of compact model and electrophysical characteristics of the device, given here, is useful for commissioning the technological process for the production of Schottky power diodes.

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