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Computer Simulation of Current Transport in GaN and AlGaN Schottky Diodes Based on Thin Surface Barrier Model

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Abstract

This paper attempts a rigorous computer simulation of the current transport in GaN and AlGaN Schottky diodes on the basis of the thin surface barrier (TSB) model recently proposed by the authors' group. First, a computer program was developed which can calculate current transport through an arbitrary potential profile of Schottky barrier by a combined mechanism of thermionic emission (TE), thermionic-field emission (TFE) and field emission (FE). Then, from the view point of the TSB model, attempts were made to fit the theoretical temperature dependent current voltage (I-V-T) curves to the measured I-V-T data taken on Ni/n-GaN and Ni/n-AlGaN Schottky diodes changing the barrier profiles and the energy depth of the surface donor. As compared with the previous poor fitting using approximate analytic formulas, excellent fitting was obtained for both forward and reverse current, confirming the validity of the TSB model as the mechanism for anomalously large leakage currents in GaN and AlGaN Schottky diodes. Best fittings for GaN and $Al_{0.26}Ga_{0.74}N$ were obtained for exponentially decaying distributions of surface defect donors with the peak density of $5x10^{18}$ cm^{-3} and $1x10^{19}$ cm^{-3}, the characteristic decay depth of 11 nm and 11.5nm and the energy depth of 0.25 eV and 0.37eV, respectively.

Keywords: GaN, AlGaN, Schottky, leakage current, deep donor, tunneling, thermionic-field emission, field emission

1. Introduction

Recently, GaN and AlGaN/GaN material systems are finding applications, not only in blue emitting lasers and LEDs, but also in a new class of devices such as high-power/high-frequency heterostructure field effect transistors (HFETs), metal- semiconductor FETs (MESFETs), power rectifiers, UV photodetectors and various gas sensors. Many of these devices utilize Schottky barriers.

However, Schottky diodes formed on GaN and AlGaN suffer from leakage currents that are many orders of magnitude lager than the prediction of standard thermionic emission (TE) model [1,2]. Large leakage adversely affects operation, power consumption, noise and reliability of devices [3]. Because of this, many papers have tried to explain I-V characteristics with limited success.

Recently, we have proposed a new thin surface barrier (TSB) model [4] assuming presence of defect donors at the surface. This could explain the measured temperature (T) -dependent current-voltage (I-V) curves systematically for the first time. However, quantitative agreement between theory and experiment was not satisfactory, most probably due to use of approximate analytic formulas only obtainable for a simple rectangular distribution of defect donors.

The purpose of this paper is to attempt a rigorous computer simulation of the current

transport in GaN and AlGaN Schottky diodes on the basis of the thin surface barrier (TSB) model. A program that can calculate current transport through Schottky barriers with arbitrary potential profiles were developed and applied. Excellent fitting was obtained, confirming the validity of the TSB model.

2. Transport Through Arbitrary Schottky Barrier

2.1 Tunneling Probability and Current Transport

According to the WKB approximation, tunneling probability, T (E_x) is given by

$$T(E_x) = \exp\left[-2\frac{\sqrt{2m^*}}{\hbar}\int_{x_1}^{x_2}\sqrt{\phi(x)-E_x}\,dx\right] \qquad (1a),$$

with $E_x = \hbar^2 k_x^{\,2} \big/ 2m^*$ (1b)

where ϕ (x) is the potential distribution, m^* is the effective mass, h is the Plank constant, x_1 and x_2 are classical turning points, and k_x is the wave number normal to the barrier. Then, the current from semiconductor to metal through the Schottky barrier can be expressed by the following general expression.

$$J = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{2q}{\hbar}\left(\frac{1}{2\pi}\right)^3\left[f_s(E)-f_m(E)\right]\times T(E_x)\left(\frac{dE_x}{dk_x}\right)dk_x dk_y dk_z \qquad (2)$$

where k_y and k_z are the wave number parallel to the Schottky barrier, and $f_s(E)$ and $f_m(E)$ are the Fermi-Dirac distribution functions for metal and semiconductor, respectively. Here, it is assumed that k_y and k_z are conserved during tunneling. By converting the double integral with respect to k_y and k_z to an integral with respect to the parallel component energy, $E_p = (h^2/2m^*)(k_y^2 + k_z^2)$, Equation (2) reduces to

$$J = \frac{4\pi q m^*}{h^3}\int_0^{\infty}T(E_x)\times\int_0^{\infty}\left[f_s(E_p+E_x)-f_m(E_p+E_x)\right]dE_p dE_x \qquad (3)$$

Since T (E_x) is an exponentially increasing function of Ex and $f_m(E_x)$ is an exponentially decreasing function, the integrand in Eq.(3) forms a Gaussian peak for tunneling at a certain energy whose energy position is temperature dependent. At sufficiently low temperature, this peak takes place at the Fermi level leading to the so-called field emission (FE). At elevated temperatures, the peak occurs above the Fermi level leading to the thermionic field emission (TFE). Equation (3) also contains the current component due electrons which travels over the barrier. This is thermionic emission (TE) component. At high temperatures, the TE process dominates. Thus, Equation (3) takes account of all the possible current transport automatically.

2.2 Comparison with Analytical Formulas by Padvani and Stratton

Previously, the TFE/TE process was discussed by using the approximate analytical formulas derived by Padvani and Stratton [5]. They are based on the Taylor expansion of the integrand of the above Eq.(3) around the energy position for the Gaussian peak.

In order to see how accurate these formulas are, I-V characteristics of a Schottky diode with

a Schottky barrier height (SBH) of 0.9 eV and a high uniform doping density of 2 x 10^{18} cm^{-3} were calculated for various temperatures by the approximate analytic formulas and by our computer program. The results are compared in **Fig.1 (a)** for the forward and reverse directions. For the forward bias region, both methods gave nearly the same linear log I-V characteristics. Padvani and Stratton [5] derived the following well-known analytic formula for the ideality factor, n_F, for the forward TFE/TE transport.

$$n_F = (E_{00} / kT)\coth(E_{00} / kT) \qquad (4a)$$

with $$E_{00} = 2q\left[N_D / 2\varepsilon\right]^{1/2} \hbar \Big/ 2(2m^*)^{1/2} \qquad (4b)$$

The values of n_F calculated using Eq. (4a) are plotted in **Fig. 1(b)** by solid lines as a function of temperature, and compared with the values obtained by our computer program (symbols). A good agreement is seen here, indicating again that analytic formulas are reasonably accurate for the forward current flow.

On the other hand, agreement was very poor for reverse leakage currents both in the small reverse bias region with TFE transport and in the large bias region with FE transport, as seen in **Fig.1 (a)**. The kinks in the analytic I-V curves are due to artificial connection of approximate TFE and TE curves. At larger biases, the reverse leakage currents by analytic formula are smaller by one to two orders of magnitude than the rigorous values. Thus, the previous analytic formulas are not accurate enough for quantitative discussion of reverse leakage currents.

3. Calculation of I-V-T Curves for TSB Model

3.1 TSB model

Our TSB model [4] is shown in **Fig. 2**. In this model, introduction of high density of unintentional defect donors near surface reduces the width of the Schottky barrier in such a way that electrons can tunnel though this barrier in both forward and reverse direction in the form of a Gaussian beam by TFE or FE mechanism depending on the temperature. As the origin of defect donors, nitrogen (N)-vacancy or its complex has been suggested.

Based on this idea, Hasegawa and Oyama [4] derived a set of approximate analytical formulas, assuming a square defect donor distribution, and made an effort to fit the theoretical I-V-T curves to experimental data. Although the procedure reproduced correct orders of magnitude for currents for the first time, quantitative agreement was not sufficiently good. An example of the result of fitting by this analytical approach is shown in **Fig.3** for a Ni/GaN diode.

3.2 Numerical Calculation of I-V-T Curves

Using our computer program for a Schottky barrier with an arbitrary potential profile, rigorous numerical calculation of I-V-T characteristics was carried out for the GaN and AlGaN Schottky diodes.

For this, the potential profile of the Schottky interface was calculated by solving the Poisson equation self-consistently, using a simulation program developed by our group. As the spatial distribution of defect donor density, a rectangular distribution and an exponentially decaying distribution schematically shown in **Fig.4 (a)** and **(b)** were considered. For the latter distribution,

the following expression was used.

$$N_{deep}(x) = N_0 \exp\left(-x/\lambda\right) \qquad (5)$$

The energy depth, E_{DD}, of the defect donor was also taken as the fitting parameter as shown in **Fig.4(c).**

4. Result of Fitting and Discussion

4.1 Fitting for a Ni/GaN Schottky Diode

As the experimental data for fitting, I-V-T data for a Ni/GaN diode reported in ref [4] was used. This is the same with the data shown in **Fig.3.** The result of fitting is shown in **Fig.5**. Here, series resistances of 0.5- 13 Ωcm^2 were introduced to fit the I-V data in high forward bias region. As seen in **Fig.5**, our simulation reproduced forward and reverse I-V-T behavior almost completely over the wide range of bias and temperature.

Let us discuss in more detail about the improvements in fittings achieved by the present computer simulation as compared with those by the previous analytic formulas by Hasegawa and Oyama [4]. For the forward bias region, the previous calculation assuming a rectangular distribution of surface defect donors showed good agreement with the experiment except for high forward bias region affected by series resistance, as seen in Fig.3. Equally good agreement was obtained over a whole forward bias region by the present computer simulation as seen in Fig.5, by including the effect of series resistance.

On the other hand, in the more important reverse bias region where large leakage currents flow, agreement between the previous calculation and the experiment was much poorer. Namely, although leakage currents of similar magnitudes with experiment could be reproduced at high reverse bias region by parameter optimization, agreements between calculation and experiment were very poor at lower reverse biases and at lower temperatures as seen in Fig.3. For example, at 150K, difference in leakage currents became nearly two orders of magnitude at around –2V. Furthermore, the artificial connection of the approximate analytic formula for the FE transport and with that for the TFE transport produced artificial kinks in the theoretical curves, as clearly seen in Fig.3. All these problems are solved by the present computer simulation. Thus, it can be concluded that much better agreement between theory and experiment could be achieved by the present computer simulation.

However, in order to achieve such good fitting for both forward and reverse directions simultaneously, it was also noted that defect donors should have specific features. Namely, for lower forward bias region and for reverse bias region, the experimental data could be reproduced only by assuming that the defect donor is a deep donor with an exponentially decaying spatial distribution. E_{DD} should be larger than 0.2 eV and below 0.35 eV to obtain reasonable fitting. The best fitting shown in Fig.5 was obtained by a set of values for SBH, N_0, λ and E_{DD} of 0.85eV, 5×10^{18} cm^{-3}, 11 nm, 0.25 eV, respectively.

In our previous paper [4], we proposed that the defect donor is the N-vacancy or its related complex. Theoretically, the N-vacancy has been reported to act as a shallow donor [6,7], or as an s-like deep donor with E_{DD} of about 0.3 eV [8]. Experimentally, our C-V measurements for various GaN metal-insulator-semiconductor (MIS) structures [9] detected a discrete surface state peak at E_{DD}= 0.3eV – 0.4 eV. Thus, the present result seems to be in agreement with the s-like donor model and our previous result.

4.2 Fitting for a Ni/AlGaN Schottky Diode

The I-V-T characteristics of AlGaN Schottky diodes were also investigated. As the experimental data, those for a Ni/AlGaN diode reported in ref. [10] were used, which showed large reverse leakage currents with strong bias dependence and very small temperature dependence, as shown in **Fig.6**. The result of fitting is also shown in **Fig.6.** Again, good fitting was possible only for an exponentially decaying distribution of deep donor. We used E_{DD} = 0.37 eV obtained by our transient measurements on gateless AlGaN/GaN HFETs [10]. The best fitting result in **Fig. 6** corresponds to SBH = 1.1 eV, N_0 = 1.0 x 10^{19} cm^{-3} and λ = 11.5 nm. An extremely high density of the defect donors seems to be produced near surface, resulting in highly anomalous I-V-T characteristics. The origin of the defect donor seems again to be N-vacancy or its complex [10].

5. Conclusion

Attempts were made to perform a rigorous computer simulation of the current transport in GaN and AlGaN Schottky diodes on the basis of the thin surface barrier (TSB) model. The developed computer program allows calculation of TFE/FE/TE current transport through an arbitrary Schottky barrier. Excellent fitting to experimental data was obtained for both forward and reverse I-V-T characteristics of Ni/n-GaN and Ni/n-AlGaN Schottky diodes, confirming the basic validity of the TSB model as the mechanism for anomalously large leakage currents. Best fittings for GaN and $Al_{0.26}Ga_{0.74}N$ were obtained for exponentially decaying distributions of surface defect donors with the peak density of 5x10^{18} $cm^{-3}$and 1x10^{19} cm^{-3}, the characteristic decay depth of 11 nm and 11.5nm and the energy depth of 0.25 eV and 0.37eV, respectively.

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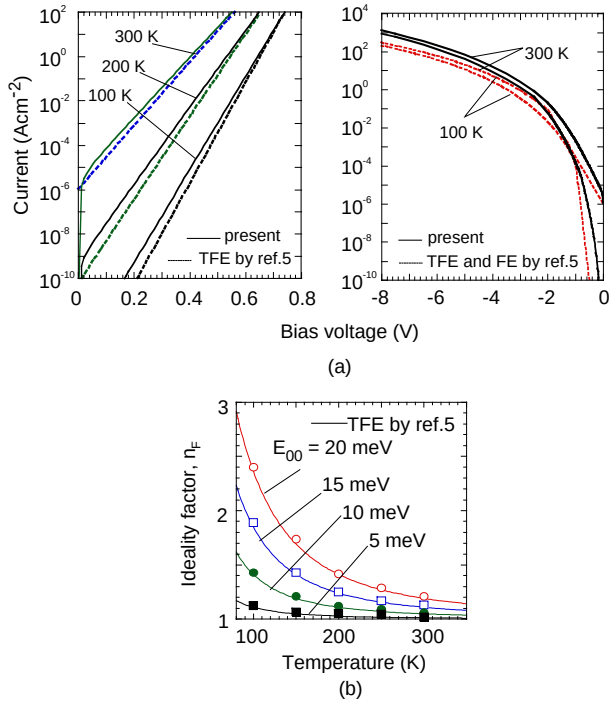

Fig.1 (a) The calculated I-V-T curves of a Schottky diode with a barrier height of 0.9 eV and a high uniform doping density of 2 x 10^{18} cm^{-3} by the approximate FE/TFE analytic formulas and by the present numerical method. (b) The ideality factor, n_F, calculated by Eq. (4) for the forward TFE/TE transport (solid lines) and by the present simulation (symbols).

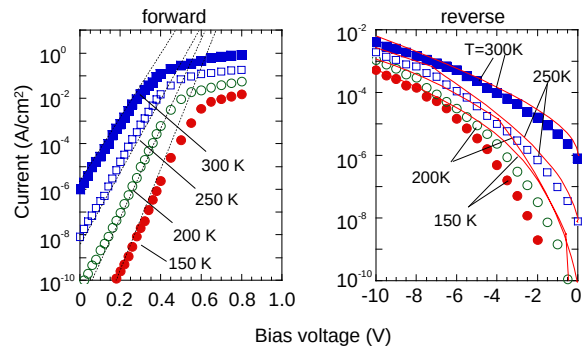

Fig.3 An example of I-V-T curves of Ni/n-GaN diodes and a result of fitting by the FE/TFE analytic approach.

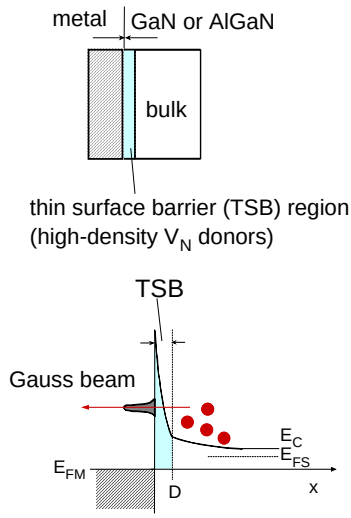

Fig.2 A schematic illustration of thin surface barrier (TSB) model.

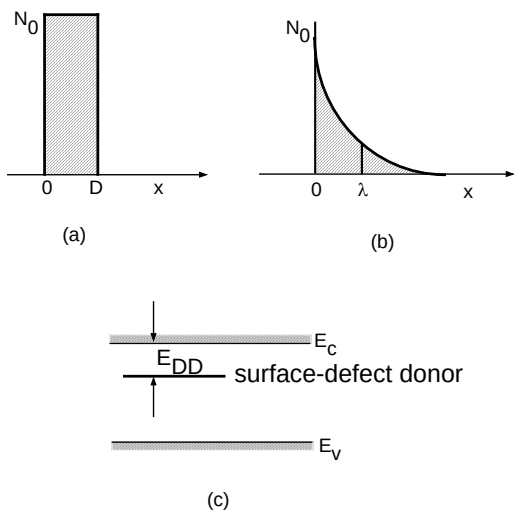

Fig.4 Schematic illustrations of (a) a rectangular and (b) an exponentially decaying distributions of defect donor density, and (c) the defect donor level.

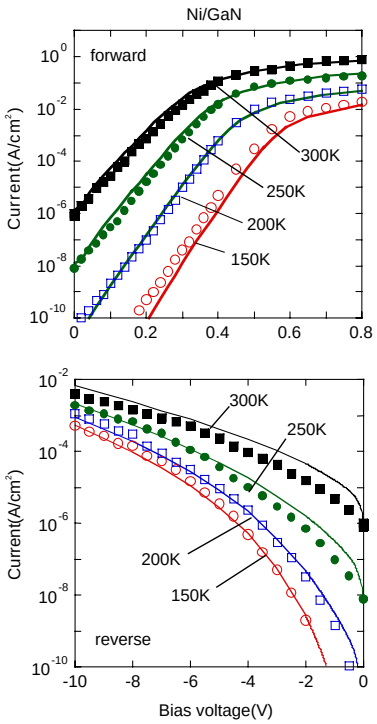

Fig.5 The experimental I-V-T curves of a Ni/n-GaN diode and the calculated ones by the present computer simulation.

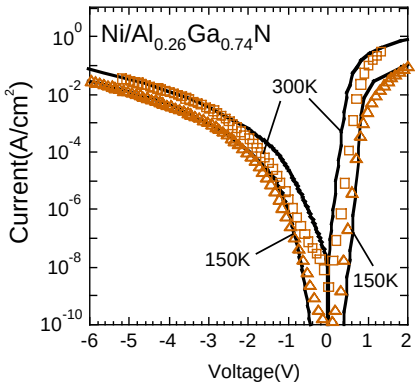

Fig.6 The experimental I-V-T curves of a Ni/n-$Al_{0.26}Ga_{0.74}N$ diode and the fitting result by the present computer simulation.