Thermionic field emission in GaN nanoFET Schottky barriers

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Abstract
A mathematical stability approach that enables the evaluation of the multivariate thermionic field emission parameters at Schottky barriers is presented. The method is general, requiring only the effective mass and relative dielectric constant for a given semiconductor. The approach is demonstrated in a first-time analysis of the barrier heights, tunneling probabilities and potential drops for changes in the Schottky barriers of gallium nitride nano-field effect transistors in a long-duration heavy ion radiation extreme environment. The investigation yielded fundamental insights into behavior that would be challenging to predict a priori.

Nanowire, nanotube and graphene nanocircuits operate as Schottky barrier devices, in which functional capability is achieved through barrier manipulation [1–3]. The general theory for Schottky barriers based on a WKB description of transport through an arbitrarily shaped Schottky barrier was developed by Sze [4], Stratton [5] and Crowell [6] among others. It has commonly been used in one of its mathematically tractable regimes, thermionic emission (TE) transport with $E > E_{\text{barrier}}$, or ohmic contact/field emission (FE) with tunneling through an electron transparent barrier. The early work on thermionic field emission (TFE) transport with a substantial but not exclusive tunneling component has been recently revisited [7, 8], as the high current densities and resulting high carrier concentrations reported in reduced dimensionality devices [9–12] indicate that they may operate in the TFE regime [6]. TFE regime analysis is difficult due to its multivariate nature. The present work presents a simple self-consistent mathematical stability approach that enables determination of the major TFE fitting parameters. It also provides a new fundamental picture of how the fitting parameters approach the TFE regime limits. The stability approach is demonstrated in a first-time analysis of the barrier heights, tunneling probabilities and potential drops for a unique dataset: changes in the Schottky barriers of gallium nitride nano-field effect transistors in a long-duration heavy ion radiation extreme environment. This investigation yielded fundamental insights into nanocircuit behavior in an extreme environment that would be challenging to predict a priori.

A reverse TFE $I-V$ curve was generated using known (generation) values for temperature $T$, carrier concentration $n$ and effective barrier height $q\phi_{\text{Bar}}$. Fits performed on the generated curve using the Levenberg–Marquardt algorithm [13] were used to identify stable parameter ranges. When the TFE model was used to fit experimental data within the identified parameter ranges, a stable solution resulted that was optimized using a least squares fit. The asymmetric Schottky barriers and carrier concentration were then determined, and a temperature dependence investigation was performed. The potential drops across the Schottky barriers and also across the nanowire as a function of time in beam and $V_{\text{ext}}$ were determined, following the recent approach of Peng [7]. The potential drop investigation was performed using a full metal–semiconductor–metal (MSM) circuit formulation with reverse TFE and forward TE Schottky barriers. The transmission probabilities at each schottky barrier as a function of time in beam were also determined, following the recent approach of Zhang [8].
The equation for reverse TFE [5, 14] is

\[
J = \left[ \frac{A^* T}{k} \right] \sqrt{\frac{\pi \varepsilon_0 q}{V + \phi_{00}} \left( \frac{\phi_{00}}{\varepsilon_0} \right)} \exp \left( -\frac{q \phi_{00}}{E_0} \right) \exp \left( \frac{qV}{e'} \right),
\]

\[E_0 = \frac{q \hbar}{2} \sqrt{\frac{n}{m^* \varepsilon_0}},\]

\[e' = \frac{E_0}{(E_0/kT) - \tanh (E_0/kT)}\]

with reduced effective Richardson constant \(A^*\), temperature \(T\), effective barrier height \(q \phi_{00}\) and carrier concentration \(n\) [8]. The effective mass \(m^*\) was equal to 0.27 \(m_0\) and the relative dielectric constant \(\varepsilon_0\) was equal to 10.4 \(\varepsilon_0\) (wurtzite GaN). The reduced effective Richardson constant is a multiplicative factor in equation (1) that shifts the J–V characteristic and was therefore assigned a previously determined experimental value [15] of 14.7 A K\(^{-1}\) cm\(^{-2}\).

Fits were first performed on a generated reverse TFE J–V curve using the Levenberg–Marquardt algorithm [13], which performs a least-squares fitting for a model equation to a dataset. The goal was to identify the range of guess values for which the fit values matched the ‘hidden’ generation values as a key first step towards finding parameter ranges for stable solutions. After each successful fit of the data, the initial generation-value guesses were set farther from the correct values. Values both well above and well below the generation values were tested. When the algorithm failed to fit the data, the guess parameters were brought in closer to the generation values until the algorithm converged onto the correct parameter values once more. In this manner, a range of parameter values was found in which the fit self-consistently identified the generation parameters. Furthermore, information about how the fit failed, whether gradually, abruptly or through location of local minimum, was obtained. This is a general method that requires only effective mass and dielectric constant for a given semiconductor.

For temperature \(T\), generation values of 250–350 K were exactly reproduced by a broad range of guess values (not shown) from 200 K through 2800 K, the melting point of GaN. Fits to the TFE equation below 200 K abruptly became unstable over a narrow range of values 199.5 K through 199.0 K. As active cooling was not employed in the beam experiments, this unstable region was never reached experimentally. A temperature parameter range of 300–350 K was used to fit the experimental data using the TFE model, allowing room temperature and possibly higher behavior.

Fits to the TFE model were more restrictive for carrier concentration \(n\). Catastrophic fit-failure observed at low guess-concentrations and gradual divergence was observed at high guess-concentrations, as shown in figure 1(a). Since the precise edge of the gradual divergence region will not be known for experimental data, guess-concentrations near this region should especially be avoided. At sufficiently high guess-concentrations, the algorithm failed to fit the curve and simply returned the initial guess as the fit value, shown in figure 1(a) as the linear region with slope \(m = 1\). Fits to the TFE equation also abruptly became unstable over a narrow range of values for each generation concentration at guess-concentrations below \(10^{16.0}\) cm\(^{-3}\), consistent with the TFE condition \(kT / E_0 \sim 1\) [6, 8] for GaN. Generation values of \(10^{19.5}\) cm\(^{-3}\) and above produced spurious local minima at low guess-concentrations (not shown) that established \(n \sim 10^{19}\) cm\(^{-3}\) as the upper limit. The constraints and limits therefore identified \(10^{16.0} \sim 10^{18.5}\) cm\(^{-3}\) as the stable parameter range for TFE model fits in GaN.

Results for effective barrier height \(q \phi_{00}\) are shown in figure 1(b). The range of guess values for which the fit reproduced the generation values was broad for low barrier heights but became increasingly restrictive as barrier height increased. The fit value diverged from the generation value without immediately evident catastrophic fit-failure at low guess-barrier heights and abruptly became unstable at high guess-barrier heights, ultimately jumping to the \(m = 1\) line. The parameter range that would safely fit all effective barrier heights for a TFE mechanism was therefore restricted to 0.7–0.8 eV.

The TFE model was then used to fit the experimental data shown in figure 2 and optimized using a least squares fit within the parameter ranges identified above. The experimental data utilized in the present study was
taken from the first real-time investigations of the electronic performance of GaN nanowire nanoFETs over thirty minutes of continuous irradiation by Xenon-124 heavy ions at relativistic energies. Two GaN nanoFETs that displayed pre-irradiation (PR) Schottky barrier $I$–$V$ characteristics with different turn-on voltages ($\sim 1$ V for nanoFET1: figure 2(a) versus $\sim 11$ V for nanoFET2: figure 2(b)) were investigated. The nanoFETs were fabricated using electron beam lithography (EBL) as previously described [10]. A highly doped p-type silicon wafer ($\sim 5 \text{m} \Omega \text{cm}$) was used as the nanoFET substrate with a 100 nm layer of thermally grown silicon dioxide as the gate dielectric. The backside of the wafer was stripped of silicon dioxide using hydrofluoric acid and Ti/Au (10/70 nm) was thermally evaporated (Edward Auto306) to form the global back gate. GaN nanowires, synthesized by a catalyst-free [16] direct reaction of gallium vapor and ammonia at 850 °C, were dispersed from an ethanol solution onto the substrate. Source and drain contacts to photo-lithographically pre-fabricated contact pads were patterned using electron beam lithography (JEOL 840A SEM). After exposure to a 100 W oxygen plasma (March Instr. PX-250) for 30 s to remove any electron beam resist residue, Ti/Au (10/30 nm) was thermally evaporated for the conducting source and drain contacts. Subsequent metal lift-off was performed in acetone. The source and drain contact pads were connected by ultrasonic wedge wire bonding (West Bond 7400B) to the individual pins of a dual in-line package. Real-time $I$–$V$ characteristics were acquired during irradiation by Xenon-124 heavy ions at relativistic 127.33 MeV per nucleon beam on target energies (140 MeV per nucleon reduced by a zirconium window and a short air gap) [17]. The beam-on-target charge state was determined to be 75% 54+ (fully stripped), 23% 53+, and 2% 50–52+, calculated by GLOBAL [18]. The beam was focused to uniformly irradiate a 10 mm × 10 mm area measured from known dimensional markings on a beam-viewing scintillator plate prior to the experiments. The active nanocircuit areas were both $250 \times 250 \mu m^2$ and therefore both nanoFETs were uniformly irradiated with fluences of $5.5 \times 10^3$ ions $\mu m^{-2}$. Families of $I$–$V$ curves at gate voltages $-1$, 0 and $+1$ V were acquired at 5 min intervals that demonstrated typical GaN n-type behavior. A bias-dependent response to irradiation was not observed and therefore only the $-1$ V bias curves are shown in figure 2. The Xenon-124 beam was blocked at 31:08 and 31:10 mins, respectively.

The turn-on voltage decreased immediately upon exposure to the beam (0 min), as shown in figure 2 insets. NanoFET2 demonstrated a substantial improvement over its PR performance that required a compliance increase to 500 nA and then to 1 $\mu A$. After the initial improvement, slight increases in turn-on voltage were
Table 1. Effective barrier heights and carrier concentrations for time in beam.

|       | \(\varphi_{Bn1} \) (eV) | \(\varphi_{Bn2} \) (eV) | Log(\(n\)) forward | Log(\(n\)) reverse | \(n_{ave} \) (\(cm^{-3}\)) | \(kT/E_{ox}\) (Avg) |
|-------|--------------------------|--------------------------|----------------------|----------------------|--------------------------|---------------------|
| NanoFET1 |                          |                          |                      |                      |                          |                     |
| Pre-rad | 0.482                    | 0.482                    | 18.33                | 17.77                | 1.12E + 18               | 2.22               |
| 0      | 0.437                    | 0.437                    | 18.23                | 18.00                | 1.29E + 18               | 2.06               |
| 5      | 0.434                    | 0.434                    | 18.26                | 18.00                | 1.35E + 18               | 2.02               |
| 10     | 0.434                    | 0.434                    | 18.26                | 18.00                | 1.35E + 18               | 2.02               |
| 15     | 0.433                    | 0.433                    | 18.27                | 17.99                | 1.34E + 18               | 2.03               |
| 20     | 0.440                    | 0.440                    | 18.28                | 18.01                | 1.39E + 18               | 1.99               |
| 25     | 0.444                    | 0.444                    | 18.28                | 18.01                | 1.40E + 18               | 1.98               |
| 30     | 0.494                    | 0.494                    | 18.35                | 17.96                | 1.44E + 18               | 1.96               |
| NanoFET2 |                          |                          |                      |                      |                          |                     |
| Pre-rad | 0.420                    | 0.466                    | 16.78                | 17.73                | 0.18E + 18               | 5.53               |
| 0      | 0.458                    | N/A                      | 17.92                | N/A                  | 0.82E + 18               | 2.59               |
| 5      | 0.449                    | 0.471                    | 17.80                | 18.13                | 0.93E + 18               | 2.43               |
| 10     | 0.451                    | 0.487                    | 17.79                | 18.11                | 0.88E + 18               | 2.5               |
| 15     | 0.453                    | 0.508                    | 17.76                | 18.13                | 0.88E + 18               | 2.5               |
| 20     | 0.448                    | 0.521                    | 17.69                | 18.12                | 0.80E + 18               | 2.62               |
| 25     | 0.451                    | 0.511                    | 17.69                | 18.04                | 0.73E + 18               | 2.75               |
| 30     | 0.449                    | 0.516                    | 17.63                | 18.05                | 0.69E + 18               | 2.82               |

observed. The \(I–V\) characteristics were therefore observed to shift, initially toward lower voltages and then toward higher voltages as a function of time in beam.

Selection of the reverse TFE model was motivated by the experimental results. In a previous study [17], space charge limited and TE model fits to the experimental data were investigated, with the conclusion that these models did not reproduce the observed experimental shifts. Furthermore, the large ideality factors required by a TE model, which have been previously reported in the semiconductor nanowire literature [9], indicated that tunneling was a significant contribution. Finally, the high current densities and resulting high carrier concentrations \(\sim 10^{18} \text{ cm}^{-3}\), which have also been widely reported in the semiconductor nanowire literature [9–12], resulted in values for \(kT/E_{ox}\) that were consistent with the TFE regime [6, 14], as shown in table 1.

The values for effective barrier heights \(\varphi_{Bn1}\) and \(\varphi_{Bn2}\) and carrier densities \(n\) were therefore obtained by least squares fits of the reverse TFE model to the exponential regions of the \(I–V\) curves at low bias. The exponential and linear regions were identified for each \(I–V\) curve and individually fit, following the approach of Peng et al [7]. The experimental contact areas required to convert \(I–V\) to \(I–V\) were estimated using scanning electron microscope images (not shown). The EBL-fabricated contact areas had similar values and the smaller values were used in the present study, pending further investigation of the actual sub-surface contact environment. The contact areas were \(7.5 \times 10^5 \text{ nm}^2\) for nanoFET1 and \(5.2 \times 10^5 \text{ nm}^2\) for nanoFET2. The values for nanowires resistances \(R\) were obtained by least squares fit of an Ohmic model to the linear regions of the \(I–V\) curves at high bias. The average values were: 0.7 M\(\Omega\) for nanoFET1 and 5 M\(\Omega\) for nanoFET2, consistent with the PR device performances.

When the metal electrodes are referred to as contacts 1 and 2 [4, 7], positive bias on the contact 2 metal electrode corresponds to forward bias of the nanocircuit. In our study, contact 1 was the reverse biased Schottky barrier, modeled by reverse TFE, and contact 2 was the forward biased Schottky barrier modeled by forward TE. When a negative bias was applied to contact 2 during the voltage sweep, the nanocircuit was in reverse bias and contact 2 was the forward biased Schottky barrier modeled by reverse TE, while contact 1 was the forward biased Schottky barrier modeled by forward TE.

The experiments were carried out at room temperature. Investigation of the TFE equation (1) for its stable parameter range showed that the \(I–V\) curve shifted to the left as a function of increasing temperature. As this did not match the experimental results for the 5–30 min time periods, and as no other indications of substantially increased temperature were present, \(T = 300 \text{ K}\) was assumed.

Effective barrier heights \(\varphi_{Bn1}\) and \(\varphi_{Bn2}\) and the carrier densities \(n\) were evaluated from reverse TFE model fits as given in table 1. Both nanoFETs exhibited asymmetric (\(\varphi_{Bn1} \neq \varphi_{Bn2}\)) effective barrier heights with values \(\sim 0.4–0.5 \text{ eV}\). The TFE analysis therefore suggested that the effective barriers may be lower than previously reported values based on TE analysis of GaN nanowires [6, 10, 19]. The carrier densities \(n\) were \(\sim 10^{18} \text{ cm}^{-3}\),
consistent with previously reported experimental results for GaN nanowires [12]. The differences between the carrier density values obtained in forward and reverse bias may be due to the lack of precise information about the actual contact areas. In subsequent calculations, the arithmetic mean $n_{\text{ave}} = (n_{\text{for}} + n_{\text{rev}})/2$ was used for $n$ as a function of time in beam. The compliance changes required by the unexpected nano FET2 improvement resulted in the collection of too few data points for complete analysis at 0 and 5 min, designated as N/A in table 1.

Evaluation of effective barrier heights $q\phi_{Bn1}$ and $q\phi_{Bn2}$ and the carrier densities $n$ further enabled determination of the transmission probabilities at each Schottky barrier as a function of time in beam. The transmission probability $T_f$ appropriate [8] for the TFE mechanism is given by

$$T_f \approx \exp \left[ -\frac{kT}{E_{00}} \right] \gamma_1 \left( \zeta_b, h \right),$$

$$\gamma_1 \left( \zeta_b, h \right) = \sqrt{\zeta_b \left( \zeta_b - h \right)} - h \ln \left( \frac{\sqrt{\zeta_b} + \sqrt{\zeta_b - h}}{\sqrt{h}} \right),$$

$$\zeta_b = \frac{E_b}{kT} = \frac{q\phi_{Bn}}{kT}, \quad h = \frac{E}{kT}.$$  \hspace{1cm} (7)

$\zeta_b$ and $h$ are the normalized barrier height and carrier energy $E < E_b$, respectively. The expression for carrier concentration as an equivalent energy $E_{00}$ [8, 14] is given in equation (2).

The transmission probabilities are shown in figure 3. For the nanoFET1, the contact 1 Schottky barrier initially showed increased tunneling at lower energies, starting from the PR to 0 min transition and continuing until 15 min, as shown in figure 3(a). It then increased over the 15–30 min time period. This differed from the energy required for tunneling at the contact 2 Schottky barrier, which increased steadily (figure 3(b)).

For nanoFET2, the contact 1 and 2 Schottky barriers both showed a new ‘crossover’ effect during the PR to 0 min transition that resulted in ~20–50% transmission probabilities at lower energies (figures 3(c) and (d)). This was consistent with the unexpected improvement that required the compliance increase during the experiments. The 5 min result is shown in figure 3(d) as the unexpected improvement resulted in a collection of too few data points for reliable analysis.

The Sze–Peng [7] formulation was used to determine the potential drops $V_1$ and $V_3$ across the Schottky barriers and $V_2$ across the nanowire as a function of $V_{\text{ext}}$ and time in beam. The voltage $V_{\text{ext}} = V_{DS}$ across the entire MSM structure is the sum

$$V_1 + V_2 + V_3 = V_{\text{ext}}.$$  \hspace{1cm} (8)

Ideally, the currents across each barrier must be equal, and must be equal to the current through the nanowire.
V_{\text{ext}} = V_{1} + \text{Area}_{3} R A^{*} T \
\times \exp \left( \frac{qV_{3}}{kT} \right)
\times \text{Area}_{3}^{*} \gamma^{*} \exp \left( \frac{-q\Phi_{\text{bl2}}}{kT} \right)
+ \text{Area}_{1} \gamma \exp \left( \frac{q\Phi_{\text{bl1}}}{kT} \right)
+ \text{Area}_{1}^{*} \text{Area}_{3} \exp \left( \frac{-q\Phi_{\text{bl2}}}{kT} \right) + \text{Area}_{3}^{*} R A^{*} T^{2} \times \exp \left( \frac{qV_{3}}{kT} \right) + V_{5},
\gamma = \left\{ \pi E_{0} \text{cos} \frac{h}{kT} \right\} \left( qV_{3} + \frac{q\Phi_{\text{bl1}}}{kT} \right).
A first-time investigation of the Schottky barrier height and ‘width’ described by potential drop $V_1$ as a function of time in beam was then performed. The results indicated that the nanoFET1 $q\phi_{Bn1}$ barrier decreased in both height and ‘width’ up to 15 min and then increased, as shown in figure 5(a). NanoFET2 experienced a significant decrease in Schottky barrier ‘width’ at 0 min (5 min shown) and a slow increase up to 30 min, as shown in figure 5(b). At 30 min, the barrier ‘width’ was still less than its PR value. The nanoFET2 $q\phi_{Bn1}$ barrier height increased slightly from PR to 0 min and then remained stable. These experimental results would be challenging to predict a priori. Specific interface charge models that produce corresponding behavior are under investigation and will be published separately.

In conclusion, a mathematical stability approach that provides the ability to evaluate stable TFE parameter ranges and from them, fits to data that provide experimentally-based TFE fitting parameter values is presented. When the TFE parameters for effective barrier heights and carrier concentrations are determined, there are many valuable analyses that can be performed. In the present work, effective barrier height and individual potential drop investigations are combined with transmission probability investigations to provide fundamental insights into nanocircuit behavior in an extreme environment that would be challenging to predict a priori. The method is general, requiring only the effective mass and relative dielectric constant as inputs and can be applied to $I$–$V$ curves from any experimental situation that causes Schottky barrier variation. The work presented therefore enables analysis of experimental nanoscale contacts using a TFE mathematical description that includes both thermionic and tunneling contributions.
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