Thermionic emission or tunneling? The universal transition electric field for ideal Schottky reverse leakage current: A case study in $\beta$-Ga$_2$O$_3$

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ABSTRACT

The reverse leakage current through a Schottky barrier transitions from a thermionic emission-dominated regime to a barrier tunneling-dominated regime as the surface electric field increases. In this study, we evaluate such a transition electric field ($E_T$) in $\beta$-Ga$_2$O$_3$ using a numerical reverse leakage model. $E_T$ is found to depend on temperature but has an extremely weak dependence on the doping concentration and the barrier height; as a result, a simple empirical expression can be derived to capture this near-universal dependence of $E_T$ on temperature. With the help of a field-plate design, we observed experimentally in lightly doped Ga$_2$O$_3$ Schottky barrier diodes near-ideal bulk reverse leakage characteristics, which match well with our numerical model and that confirm the presence of the transition region. Near the transition electric field, both thermionic emission and barrier tunneling should be considered. This study provides important guidance toward accurate design and modeling of Schottky barrier diodes, which can be readily extended to other semiconductors.

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With a unique combination of an ultra-high breakdown electric field of $\sim$8 MV/cm,$^{2,3}$ a decent electron mobility of $\sim$200 cm$^2$/V·s,$^4$ an availability of melt-grown substrates,$^5$ and controllable n-type doping,$^3$ $\beta$-Ga$_2$O$_3$ is an attractive ultra-wide bandgap semiconductor material for applications demanding high power handling capability.$^6$ To date, promising performance in Ga$_2$O$_3$ devices has been demonstrated, including Schottky barrier diodes with a breakdown voltage (BV) over 2 kV,$^7$ high-voltage power transistors,$^8,9$ and RF transistors.$^{10,11,12}$

Ga$_2$O$_3$ Schottky barrier diodes (SBDs) are highly versatile. They can be used as high-speed rectifiers for efficient power regulation$^{13-19}$ and also function as UV photodetectors.$^{20,21}$ In addition, a Schottky contact is a key device building block, offering gate control for metal-semiconductor field-effect transistors (MESFETs),$^{1}$ as well as serving potentially as a p-n junction replacement for high field management.$^{20,21}$

Central among all the aforementioned functionalities is the reverse blocking capability of the Schottky barrier, which is critically dependent on the reverse leakage current. In general, the ideal total reverse leakage current ($J_{R,tot}$) through a Schottky barrier consists of the transport of electrons both above and below the top of the barrier. The former mechanism is thermionic emission ($TE$), while the latter is barrier tunneling ($BT$), which comprises thermionic-field emission ($TFE$) and field emission ($FE$).$^{22,23}$ As a result, $J_{R,tot}$ can be expressed as

$$ J_{R,tot} = J_{TE} + J_{BT}, $$

where $J_{TE}$ is the thermionic emission current and $J_{BT}$ the barrier tunneling current.

It has been widely recognized that, at a certain temperature, there should exist a transition voltage ($V_T$) or transition electric field ($E_T$), below which $TE$ dominates and above which $BT$ dominates.$^{22,23}$ $E_T$ is defined as the surface electric field where $J_{TE} = J_{BT}$, while $V_T$ is defined as the corresponding reverse-bias voltage. Knowledge about $V_T$ or $E_T$ is highly valuable since it determines the appropriate bias or electric field ranges for $TE$ and $BT$ models. However, due to the difficulty in calculating the tunneling current analytically near this transition region, there has not been a simple closed-form expression for $V_T$ or $E_T$. In previous studies, $V_T$ in $\beta$-Ga$_2$O$_3$ has been calculated...
numerically, but the dependence on the doping concentration, barrier height, and temperature is very complicated. Also, the non-monotonic temperature dependence of $V_T$ is questionable. In this study, we first show from the numerical calculation that, unlike $V_T$, $E_T$ is nearly independent of the doping concentration and the barrier height; furthermore, there exists a universal monotonic temperature dependence of $E_T$.

Experimentally, most of the previous analyses on the reverse leakage current in Ga$_2$O$_3$ SBDs use either the TE model$^{16,22}$ or the TFE model,$^{23,24}$ without considering their respective appropriate ranges. We have previous observed and verified near-ideal bulk reverse leakage current in Ga$_2$O$_3$ SBDs fabricated on bulk substrates.$^{25}$ However, due to the high doping concentration employed, the transit electric field could not be accessed in the study in Ref. 20. In this work, we fabricate SBDs on an n-Ga$_2$O$_3$ epitaxial layer, which allows us to access the surface electric field around $E_T$ with the edge leakage current sufficiently suppressed with a field-plane structure.

For the calculation of the reverse leakage current, two effects on the shape of the Schottky barrier potential should be considered: image-force lowering (IFL) and doping effects, as illustrated schematically in Figs. 1(a) and 1(b), respectively. With both effects included, the potential energy distribution of the Schottky barrier under a surface electric field $E$ is given by

$$E_s(x) = \epsilon \phi_h - E x - \frac{e^2}{16\pi\epsilon_0 x} + \frac{e^2(N_D - N_A)x^2}{2\epsilon_s},$$

where $\phi_h$ is the barrier height, $N_D - N_A$ is the net doping concentration, and $\epsilon_s = 10\epsilon_0$ is the dielectric constant of $\beta$-Ga$_2$O$_3$. Here, the Fermi-level energy in metal ($E_{Fe}$) is taken as the zero-energy level, as shown in Fig. 1(a). Due to the presence of IFL, the barrier is lowered by $\Delta\phi = \sqrt{eE/(4\pi\epsilon_0)}$, i.e., $E_{c,max} = \epsilon(\phi_h - \Delta\phi)$. Assuming a transmission probability of unity for electrons with an energy $E$ higher than $E_{c,max}/k_BT$ is given by the familiar expression,

$$J TE = A T^2 \exp \left( -\frac{\varepsilon \phi_h - \varepsilon \Delta\phi}{k_BT} \right),$$

where $A^* = 4\pi m^* k_B^2 /h^2$ is the Richardson constant.

On the other hand, including both IFL and doping effects in the calculation of the barrier tunneling current is analytically intractable, and thus, we developed a numerical approach, as presented in our previous work.$^{20}$ To obtain solely the barrier tunneling current, the upper limit of the integration in Ref. 20 should be changed to $E_{c,max}$, i.e.,

$$I_{BT} = \frac{A^* T}{k_B} \int_{E_{c,max}}^\infty T(E) \cdot \ln \left[ 1 + \exp \left( -\frac{E - E_{Fe}}{k_BT} \right) \right] dE,$$

where $T(E)$ is the transmission probability, whose expression is given in Ref. 20. A single effective mass $m^* = 0.31 m_0$ is adopted for both the Richardson constant and the tunneling effective mass in $T(E)$ due to the single-valley and near-isotropic nature of the conduction band in $\beta$-Ga$_2$O$_3$.

Figure 1 shows the calculated $I_{R,tot}$ using the numerical model and its constituent components ($I_{TE}$, $I_{BT}$). Here, we have temporality neglected the doping effect to compare with the analytical TE and TFE models derived by Murphy and Good,$^{22}$ which consider only the IFL. It can be seen that the calculated $I_{R,tot}$ from our numerical model agrees well with Murphy and Good’s models within their respective applicable ranges, indicating that our numerical model is valid. It is worth noting that Murphy and Good’s TE model actually includes both the TE and BT currents despite what the name suggests, and thus, it comes as no surprise that a match with $I_{R,tot}$ is observed, rather than with $I_{TE}$.

With the numerical model established, the transition electric field $E_T$ can be calculated by equating $I_{TE}$ with $I_{BT}$. Figure 2(a) shows the calculated $E_T$ as a function of $N_{D}/N_A$ at different temperatures, at a barrier height of 1.2 eV. $E_T$ is primarily a function of temperature and has a very weak dependence on $N_{D}/N_A$. It is nearly constant when $N_{D}/N_A < 10^{17}$ cm$^{-3}$ and only increases slightly (<0.08 MV/cm) when $N_{D}/N_A$ approaches $2 \times 10^{18}$ cm$^{-3}$, indicating that the influence of the doping effect is near negligible. The surface electric field at zero bias ($E_0$) is also calculated by the familiar expression: $E_0 = \sqrt{2(N_D - N_A)(eV_{bi,0} - k_BT)/\epsilon_s}$, where $V_{bi,0}$ is the built-in potential at zero bias. If $E_0$ is larger than $E_T$, $I_{R,tot}$ would be dominated by barrier tunneling, as in the case of the SBD we reported in Ref. 20. This illustrates the superiority of using the surface electric field instead of the reverse bias as the variable to characterize the transition region, as $V_T$ would have a large dependence on $N_{D}/N_A$ even with a constant $E_T$.

Knowing the weak dependence on the doping concentration, we calculate $E_T$ as a function of temperature without considering the doping effect, as shown in Fig. 2(b). Here, we examine the influence of the barrier height ranging from 0.5–2.0 eV. Interestingly, there is a negligible dependence on the barrier height from 100 K to 800 K. This is because near the transition electric field, the majority of contribution to $I_{BT}$ arises from the tunneling electrons with energy $E$ close to $E_{c,max}$, such that the natural log term in Eq. (4) can be simply replaced by $\exp \left( -\frac{E_{Fe}}{k_BT} \right)$, as long as the barrier height is not too small.
Consequently, it can be shown that $J_{BT} \propto \exp\left(-e\phi_B/k_BT\right)$, and thus, the condition of $J_{BT} = J_{TE}$ does not depend on the barrier height. Below 100 K, however, there exists a sharp transition of $E_T$ to zero at some “transition” temperature, depending on the barrier height. This comes from the fact that the contribution of tunneling electrons with energy $E$ close to $E_F$ can no longer be neglected, leading to more complicated dependence on the barrier height in $J_{BT}$. Because of the exponential decrease in $J_{TE}$ at cryogenic temperatures, to match $J_{BT}$ with $J_{TE}$, the required $E_T$ is very low, <0.06 MV/cm. Also, with $N_D-N_A \geq 1 \times 10^{16}$ cm$^{-3}$ in practice, the value of $E_T$ around this transition region would already be lower than $E_F$, rendering it unobservable.

Due to the negligible dependence on the barrier height and very weak dependence on the doping concentration, we can describe $E_T$ in $\beta$-Ga$_2$O$_3$ with a near-universal empirical temperature dependence as obtained from a quadratic fitting to the numerical calculation in Fig. 2(b),

$$E_T = 0.70 \cdot T^2 + 780 \cdot T - 3.0 \times 10^4 \frac{V}{cm},$$

(5)

where $T$ is in units of K. Eq. (5) is valid within the temperature range of 100–800 K and a barrier-height range of 0.5–2.5 eV, with maximum errors of 0.01 MV/cm for $E_T$ < 100 K and 0.08 MV/cm for $N_D-N_A \leq 2 \times 10^{18}$ cm$^{-3}$.

To verify the existence of the transition region experimentally, we fabricated field-plated SBDs on a (001) Ga$_2$O$_3$ epitaxial wafer grown by halide vapor phase epitaxy (HVPE), as schematically shown in Fig. 3(a). The field plate length is designed to be 30 nm for the purpose of suppressing the electric field crowding at the anode edge. The cathode Ohmic contact is based on Ti/Au (50/100 nm), while the anode Schottky contact is based on Ni/Au (40/150 nm). The fabrication processes for the formation of cathode and anode contacts were the same as described in Ref. 31. After the anode formation, a 31 nm Al$_2$O$_3$ was deposited by atomic layer deposition (ALD) at 300 °C, acting as the dielectric for the field plate. Finally, a contact hole was etched, followed by the deposition of the field plate, which comprises a stack of Ni/Ti/Al/Pt (30/10/80/20 nm).

Temperature-dependent capacitance–voltage ($C$–$V$) measurements were performed on co-fabricated SBDs without the field plate. Figure 3(b) shows the extracted doping profile, which shows an average $N_D-N_A$ value of $\sim 7 \times 10^{15} \text{cm}^{-3}$ in the Si-doped $n^+$ drift layer. The $1/C^2$–$V$ plot is shown in the inset, from which the values of $V_{BD}$ are extracted to be 1.10 V at 25 °C and 0.92 V at 200 °C, corresponding to barrier heights of 1.27 eV and 1.21 eV, respectively (also see Figs. 4 and 7).

Figure 4(a) shows the measured temperature-dependent forward current–voltage ($I$–$V$) characteristics. Since the doping concentration is low, the depletion width at zero bias is $\sim 0.4 \mu$m. In this case, the TE model is inappropriate for the analysis of the forward $I$–$V$ characteristics since the electron transport through the depletion region cannot be assumed ballistic, especially considering that the mobility of Ga$_2$O$_3$ is not very high. Therefore, we analyze the data using the thermionic emission-diffusion (TED) model, which considers the drift-
diffusion transport in the depletion region. In the calculations, the temperature-dependent drift mobility model in Ref. 3 is used with the Hall factor considered. The constant of proportionality is adjusted to match the Hall mobility of 145 cm$^2$/V·s measured at 25°C on a similar wafer.

The extracted barrier heights and ideality factors ($n$) from the TED model at each temperature are plotted in Fig. 4(b). The ideality factor is 1.02 at 25°C and decreases to below 1.01 beyond 100°C, indicating a very good Schottky contact quality. The image-force controlled ideality factor limit ($n_{IF}$) is calculated to be 1.007 using the standard method. It can be seen that the extracted ideality factor approaches $n_{IF}$ beyond 75°C, further suggesting a near-ideal interface. Both the apparent barrier height and the barrier height after image-force (IF) correction ($\Delta V_{BT,IF}$) are plotted. The IF-corrected barrier height is around 1.20 eV.

To verify the effect of the field plate in suppressing the edge leakage current, temperature-dependent reverse $I$–$V$ measurements were performed on both non-field-plated and field-plated SBDs on the same wafer, as shown in Figs. 5(a) and 5(b), respectively. Without the field plate, the SBDs exhibit a large, near temperature-independent reverse leakage current below 100°C. As have been pointed out in our previous report, such a leakage behavior is characteristic of field-emission dominated edge leakage current due to electric-field crowding at the anode edge. On the other hand, the leakage current in SBDs with FP is much reduced, suggesting that the FP structure is effective in suppressing the edge electric-field crowding. Note that between −200 V and −100 V, there still exists a very low level of leakage current at 25−75°C, which does not show a much temperature dependence, suggesting that there is still some edge leakage current not completely eliminated. However, considering the very low magnitude ($<10^{-11}$ A/cm²) and the weak temperature dependence, it will not significantly “pollute” the uniform bulk leakage current from 100°C to 200°C, which we will model using our numerical models.

Figure 6 shows the temperature-dependent reverse leakage current as a function of the surface electric field, i.e., $J$–$E$ characteristics. The reverse leakage characteristics from 100°C to 200°C can be well-fitted with the calculated total reverse leakage current ($J_{BT,cal}$) using our numerical model [Eqs. (1)–(4)], with the barrier height as the only fitting parameter at each temperature. The individual components of $J_{BT,cal}$, i.e., $J_{TE}$ and $J_{BT}$, are also plotted in Fig. 6. While $J_{TE}$ matches with the measured data at the lower end of $E$ and $J_{BT}$ at the higher end of $E$, neither $J_{TE}$ nor $J_{BT}$ alone can capture well the field dependence throughout the electric-field range (0.07−0.69 MV/cm). These results strongly suggest the presence of the transition regime, where both $J_{TE}$ and $J_{BT}$ are important.

The validity of the fitting depends critically on the fact that the measured bulk reverse leakage current is near ideal. A good check would be comparing the barrier height values extracted from the reverse leakage characteristics with those extracted from other methods. Figure 7 shows such comparisons. The barrier height values...
extracted from forward $I$–$V$, reverse $I$–$V$, and $C$–$V$ measurements exhibit good agreement. These provide further evidence that the measured reverse leakage current is near ideal, which, in turn, corroborates the identifications of the transition region from the data fitting in Fig. 6. The barrier heights extracted from $C$–$V$ measurements are slightly larger than those from the $I$–$V$ methods, especially at lower temperatures. This behavior is commonly observed (see, e.g., Ref. 19) and could be due to the presence of barrier height inhomogeneity and/or uncertainty of the doping concentration close to the Schottky contact interface.

In conclusion, the transition electric field ($E_T$) separating the thermionic emission- and barrier tunneling-dominated reverse leakage regimes is calculated in $\beta$-Ga$_2$O$_3$ Schottky barrier diodes, by using a numerical reverse leakage model. $E_T$ is shown to have a very weak dependence on the doping concentration and the barrier height. A near-universal expression for $E_T$ is obtained, which is valid for wide temperature, doping, and barrier-height ranges in $\beta$-Ga$_2$O$_3$ SBDs. Experimentally, we confirmed the presence of the transition region in field-plated Ga$_2$O$_3$ SBDs, which shows near-ideal bulk reverse leakage current well-matched with our numerical model. With the knowledge about the transition electric field, the long-standing confusion about whether the thermionic emission model or the tunneling model should be used is lifted: if the surface electric field is much lower than $E_T$, the thermionic emission model can be used; conversely, the barrier tunneling model should be employed. Near $E_T$, it is important to consider both models. These results and methodologies are highly valuable for the design of functional Schottky barriers in nearly all semiconductors that rely on the precise knowledge about the reverse leakage current.

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**DATA AVAILABILITY**

The data that support the findings of this study are available within this article.

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