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ABSTRACT

Vertical heterojunction NiO/ β n-Ga₂O/n⁺ Ga₂O₃ rectifiers employing NiO layer extension beyond the rectifying contact for edge termination exhibit breakdown voltages (V_B) up to 4.7 kV with a power figure-of-merits, V_B²/R_{ON} of 2 GW·cm⁻², where R_{ON} is the on-state resistance (11.3 m Ω cm²). Conventional rectifiers fabricated on the same wafers without NiO showed V_B values of 840 V and a power figure-of-merit of 0.11 GW cm⁻². Optimization of the design of the two-layer NiO doping and thickness and also the extension beyond the rectifying contact by TCAD showed that the peak electric field at the edge of the rectifying contact could be significantly reduced. The leakage current density before breakdown was 144 mA/cm², the forward current density was 0.8 kA/cm² at 12 V, and the turn-on voltage was in the range of 2.2–2.4 V compared to 0.8 V without NiO. Transmission electron microscopy showed sharp interfaces between NiO and epitaxial Ga₂O₃ and a small amount of disorder from the sputtering process.

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Recently, there is significant interest in the development of wide and ultra-wide bandgap semiconductors for power electronics applications to overcome the high on-state resistances and limited power capabilities of Si-based electronics.^{1–10} In Si-based power electronics, nearly 10% of electricity in the U.S. is wasted on power conversion, and reducing these losses can help reduce reliance on fossil fueled power plants. The reduction of resistive losses and higher energy conversion efficiency of commercialized SiC and GaN can improve both the power density and efficiency of systems controlling power switching.¹⁻⁷ Further improvements in the power figure-of-merit (FOM) should be possible with ultra-wide bandgap semiconductors such as diamond, Ga₂O₃, and AlN.⁸⁻¹⁴ In particular, there has been significant progress in monoclinic β -Ga₂O₃, which shows both materials¹⁵ 🍄 and economic¹¹ benefits and is commercially available in a high quality large area substrate form using well-established melt crystal growth methods.^{9,10} Lateral β -Ga₂O₃-based devices with breakdown voltage up to 8 kV (Ref. 15) and critical breakdown fields exceeding the theoretical limits of SiC and GaN have been reported.^{15,32} Vertical geometry devices are also attractive due to their larger current-carrying capability, and breakdown voltages >2 kV have been reported for β -Ga₂O₃ vertical rectifiers involving planar or trench metal-oxide-semiconductor (MOS) approaches.^{20,47,48} A recent report

has demonstrated up to $6 \, kV$ breakdown using a vertical structure with a deep trench of SiO₂ to provide edge termination.⁴⁹

With conventional, planar vertical geometry Ga₂O₃ rectifiers, the maximum electric field occurs at the edge of the rectifying contact, and thermionic field emission (TFE)-dominated leakage limits performance.²² The electric field concentration at the edge of the gate electrode is several times higher than under the center region of the contact.^{8,9,30} This has led to research on trench MOS approaches, where the maximum field occurs at the trench bottom and the use of a dielectric decreases the leakage current.^{8,20,22,29,47} A disadvantage is additional process complexity and reduced forward current density. Junction barrier Schottky (JBS) rectifiers have similar issues.9, Irrespective of the edge-termination structure, the total length of termination along the surface plays a role in increasing the breakdown voltage.³⁰ Typically for SiC power devices, it is difficult to ensure high breakdown voltage and process robustness when the termination region is shorter than 3-5 times the thickness of the voltage-blocking layer.3

The lack of shallow p-type dopants for β -Ga₂O₃ has created interest in integration of n-type Ga₂O₃ with p-type NiO for vertical p–n heterojunction power diodes.^{33,36–46} These typically show smaller leakage current than conventional planar rectifiers and also have larger

turn-on voltages.^{38–42} The minority carrier nature of these devices should allow lower on-resistances and better on-state performance. Sputtered NiO_x is polycrystalline with a bandgap of ~3.7–4.0 eV and controllable p-type doping.⁵⁰ NiO/ β -Ga₂O₃ JBS diodes with area 100 × 100 μ m² have demonstrated a V_B of 1715 V and a R_{ON} of 3.45 mΩ cm² for a Baliga's figure of merit of 0.85 GW cm⁻². The highest reported values are a static V_B of 2.41 kV (Ref. 51) and a specific onresistance of 1.12 mΩ cm², producing a FOM of 5.18 GW cm^{2.51} For larger devices, a JBS diode with area 1 × 1 mm2 showed a forward current of 5 A and a breakdown voltage of 700 V (FOM 64 MW/cm²).²³ For a 9-mm² heterojunction rectifier, a surge current of 45 A was reported with over 1 × 10⁶ times dynamic breakdown at a 1.2-kV peak overvoltage.⁴²

In this paper, we show that, with guidance from Technology Computer-Aided Design (TCAD) simulations in designing the NiO layer doping and thickness and extension beyond the rectifying contact, plus careful control of sputtering parameters, it is possible to achieve 4.7 kV V_B in vertical planar NiO/Ga₂O₃ rectifiers and a FOM of 2 GW cm⁻². These devices are processed without the complications of trench etching and subsequent dielectric deposition.

We first ran TCAD simulations from the Silvaco Atlas code to examine the effect of various device structures with and without NiO and then focused on differences between a single layer of NiO and a bilayer. The latter was used to optimize the contact resistance and field profiles. The NiO doping concentration (10^{15} – 1×10^{19} cm⁻³), thicknesses (10, 20, 40, 60, and 80 nm), and single vs double layers at constant thickness were variables in both simulations and subsequent fabricated devices. The distance $(1-15 \,\mu\text{m})$ of a NiO guard ring from the rectifying contact was also simulated. According to our previous experiments, the energy bandgap and the hole mobility of NiO were set to be 3.8 eV and 0.5 cm²/V s, respectively. Based on the simulation results as guidance, we fabricated the structures I-IV that are shown schematically in Fig. 1. By extending NiO beyond the edge of the metal contact, simulations and subsequent experimental data showed that this provided a type of guard ring effect in spreading the electric field crowding at the edge of the diodes, and thus, structure II had superior breakdown voltages to structure I. While the electric field distributions of structures II and III were similar, experimentally, we found that a large area of NiO due to full extension of the conducting NiO to the edge of the device caused high leakage current. Structure IV did not improve the electric field in the TCAD simulation or in the experimental V_B. Figure S1 in the supplementary material shows more details in a schematic of the one- and two-NiO layer approaches, the metal and NiO thicknesses, and the O2/Ar sputtering ratios used to control the p-doping level in NiO.

Based on guidance from the simulations, we then fabricated vertical rectifiers on structures consisting of a thick, lightly doped epitaxial layer on a conducting substrate. The drift region of the material consisted of a 10 μ m thick, lightly Si doped epitaxial layer grown by halide vapor phase epitaxy (HVPE) with a carrier concentration of 2 × 10¹⁶ cm⁻³, grown on a (001) surface orientation Sn-doped β -Ga₂O₃ single crystal (Novel Crystal Technology, Japan). A full area Ti/Au backside Ohmic contact was formed by e-beam evaporation and was annealed at 550 °C for 1 min under N₂ ambient.⁴⁸ NiO was deposited by magnetron sputtering at 3 mTorr and 150 W of 13.56 MHz power using two separate targets operated at the same time to double the

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FIG. 1. Different structures simulated in the TCAD program. These included the extent of NiO extension beyond the rectifying contact, width, and separation of the NiO guard ring from rectifying contact, thickness, and doping in NiO and one layer vs two layers of NiO with different doping in each. Based on the TCAD, structures I, II, and III were then fabricated with different thicknesses of the NiO layers.

deposition rate to around 0.2 Å s⁻¹. Calibration of the doping and mobility was made from Hall measurements on a thick layer (60 nm) of NiO deposited on quartz. The Ar/O₂ ratio was used to control the doping in NiO in the range 2×10^{18} – 3×10^{19} cm⁻³ with mobility $< 1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, and we used both single and double layers with two different doping concentrations, the first, lighter-doped layer on top of Ga₂O₃ to enhance breakdown while a subsequent more heavily doped layer on top of that was used to minimize the contact resistance. The Ni/Au contact metal (100 μ m diameter) was deposited onto the NiO layer after annealing at 300 °C under O₂ ambient. Compared to typical NiO thicknesses of 300–500 nm, we used ultra-thin layers. Previous simulations reported in the literature show that while the heterojunctions diodes will have higher turn-on voltage, they should exhibit higher reverse breakdown than conventional Schottky rectifiers.⁵²

The top layer NiO thickness was held constant at 10 nm while the bottom layer of NiO thickness varied from 10 to 80 nm. The best simulation results (and subsequent experimental, results, as shown in the supplementary material, Table S1) were obtained on structure II, shown in Fig. 2, which has the limited extension of the NiO beyond the rectifying contact to provide edge termination. To summarize the link between the TCAD simulation results and the experimental structures, (i) we found that a single layer of NiO always produced higher fields and lower simulated breakdown than a bi-layer when the latter structure was optimized to have higher doping in the upper layer and lower doping in the layer directly on top of the Ga₂O₃. Increasing the doping concentration of the NiO layer in contact with the Ni/Au electrode reduced the maximum electric field at the contact edge. Similarly, reducing the doping concentration of the lower NiO layer in contact with Ga2O3 also reduced field crowding; (ii) the extension of NiO beyond Ni/Au also increased the breakdown voltage, but there was no improvement beyond an extension of 5 μ m (Fig. S1), similar to the general trends reported for SiC rectifiers;^{3,5} (iii) increasing the thickness of the NiO was deleterious to breakdown beyond a total of 20 nm for the bi-layer, as the maximum field at the surface increased. The TCAD results were then used to guide the experimental device design.

A 20/80 nm Ni/Au Schottky contact was deposited with E-beam after lithographic patterning followed by standard acetone liftoff. Figure 2 also shows how NiO is able to reduce the field at the edge of the rectifying contact, as predicted from the TCAD simulations. Those simulations also showed that the electric field decreases with lower



FIG. 2. (a) Schematic of the optimized NiO/Ga₂O₃ heterojunction rectifier.(b) TCAD simulations showing the reduction in the electric field in Ga₂O₃ at the edge of the contact with NiO.

doping concentrations and with smaller thickness, and the electric field in the NiO film increased while the electric field in Ga_2O_3 decreased. However, this is also a function of doping and guidance on what to use experimentally was obtained from the simulations.

The current-voltage (I-V) characteristics were recorded with a Tektronix 370-A curve tracer and a 371-B curve tracer, and Agilent 4156C was used for forward and reverse current measurements over the temperature range of 300-600 K on a temperature-controlled stage. The forward direction was dominated by the thermionic emission (TE) current, while in the reverse direction, the thermionic field emission (TFE) and tunneling currents played an important role at high reverse bias.^{53,54} The reverse breakdown voltage was defined as the bias for a reverse current reaching 0.1 A cm², which has been standard for previous studies.^{42,51} Many devices (5-10) were measured for each design and typically showed V_B values within a few percent of each other within an area of 0.5 cm². The breakdown values were overwhelmingly repeatable, and only a few tests (around 5%) resulted in destructive reverse breakdown. This is consistent with our previous observations,^{14,24,26} in that edge terminated devices are much more robust than unterminated rectifiers.

For transmission electron microscopy (TEM) imaging, crosssectional TEM samples of the NiO/ β -Ga₂O₃ heterostructures were prepared along the [100] zone axis (β -Ga₂O₃) using a FEI Helios Dualbeam Nanolab 600 focused ion beam (FIB) system. High resolution TEM (HRTEM) imaging of the NiO/ β -Ga₂O₃ interface structure was carried out using a 200 kV Talos F200i (Thermo Scientific) equipped with a Ceta 16 M camera. Typical images are shown in Fig. 3. Figure 3(a) shows a HRTEM image of the full diode structure, consisting of the top electrode (Au, Ni), p-type NiO, and n-type β -Ga₂O₃ from top to bottom, recorded along the [100] projection with respect to β -Ga₂O₃. Near-surface damage is present within the top 10 nm of the Si-doped β -Ga₂O₃ layer, as evidenced by the image contrast change in Fig. 3(a). This is likely due to the energetic sputtering process for the NiO overlayer. However, a high magnification HRTEM image in Fig. 3(b) demonstrates that the NiO/ β -Ga₂O₃ interface is atomically abrupt and the β -Ga₂O₃ near the heterointerface is fairly pristine in the absence of extended defects (e.g., dislocations).

The reverse I-V characteristics from a selection of rectifiers are shown in Fig. 4. These were measured in a Fluorinert atmosphere at 25 °C. The experimental values of breakdown and on-resistance for single layer and double layer NiO structures are shown in Table S1 of the supplementary material. The double layer structures exhibited much larger breakdown voltages than the dingle layer structures, showing the benefit of optimizing the field profile. The maximum value of ${\sim}4.7\,\mathrm{kV}$ was obtained for a two-layer NiO structure with respective thicknesses of 10/10 nm and the respective doping of 2.6 $\times 10^{19}/3.5 \times 10^{18}$ cm⁻³. Increasing the thickness of the NiO reduced the V_B and was 2.5 kV for 80 nm NiO. This is consistent with the improved performance of other devices using thinner NiO.⁵¹ The metal gate rectifier without NiO showed a $V_{\rm B}$ of ${\sim}840\,V$ for this contact dimension of 100 μ m. The maximum value of V_B for the heterojunction rectifier is about twice that of reported previously,⁵¹ and the data suggest that even higher values could be obtained with further optimization. For the other device designs, for structure I, the V_B was <2 kV in all cases, while for structure III, the leakage current was large (>1 mA/cm² at -100 V). For structure IV, the V_B was similar to that of the simple NiO layer extension and the added guard rings made no improvement. The simplicity of the optimized device design



FIG. 3. (a) Low magnification HRTEM image of the NiO/ β -Ga₂O₃ heterostructure with the top Au/Ni electrode. (b) High magnification HRTEM image of the interface between NiO and β -Ga₂O₃, showing the sharp interface. Structural damage near the surface of β -Ga₂O₃, marked by the blue arrows in (a) and (b), is observed that is evidenced by the image contrast change. This damage is likely induced by the energetic deposition process of the NiO overlayer, while the β -Ga₂O₃ top layer is pristine otherwise as shown in (b).

and straightforward processing without the need for trenches makes this an attractive option.

The forward I-V characteristics are shown in Fig. 5 for the heterojunction rectifiers with different NiO thicknesses. Compared to the turn-on voltage of 0.8 V for the conventional metal rectifier, those for the heterojunctions are in the range 2.2-2.4 V but with similar current densities at these higher forward biases. The leakage current density before breakdown was 144 mA/cm², and the forward current density was 0.8 kA/cm² at 12 V. Table I shows a compilation of the R_{ON} and power figure-of-merit values for the conventional rectifier and for the heterojunction rectifiers with different thicknesses of NiO. While the R_{ON} values for the latter are slightly higher than for the conventional rectifier, optimization of the doping/thickness of NiO can minimize this difference.⁵¹ In our case, the lateral spread resistance of the NiO layer for 20 nm thickness is $\sim 10^4 \Omega$, significantly larger than the device on-resistance. This means there is insignificant lateral expansion of the conductive area for this device design. The power figure-of-merit of $2 \,\text{GW} \,\text{cm}^{-2}$ is still well short of the theoretical maximum of $\sim 34 \,\text{GW}$ cm⁻² and shows there is still room to optimize the edge termination and defect density in the drift layer. Figure 6 shows the on-state



FIG. 4. Reverse I–V characteristics from conventional Ga₂O₃ and double NiO layer NiO/Ga₂O₃ heterojunction rectifiers in which the top, heavily doped NiO thickness was constant at 10 nm while the lower, lighter doped NiO was varied from 10 to 80 nm. The arrows mark where breakdown occurs to guide the eye. This is slightly different than the definition used to standardize V_B .

resistances and forward current densities for these same devices with current densities >10 A cm⁻² even at relatively low bias.

Figure 7 shows a compilation of R_{on} vs V_B results reported in the literature for a conventional Schottky barrier or JBS rectifiers and NiO/Ga₂O₃ heterojunction rectifiers, along with the theoretical lines for different wide bandgap and ultra-wide bandgap semiconductors. This work shows the potential of Ga₂O₃ to achieve values comparable to the limits of GaN and SiC. The future work should continue to focus on defect reduction in the Ga₂O₃ epilayers, low damage edge termination methods, transition to larger device areas, and the reliability of devices under realistic operating conditions.

In summary, we present a double-layer NiO/ β -Ga₂O₃ p-n heterojunction diode, which exhibits high performance breakdown voltage



FIG. 5. Forward I–V characteristics from conventional Ga₂O₃ and double layer NiO/ Ga₂O₃ heterojunction rectifiers with different NiO thicknesses.

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Parameter	Ga ₂ O ₃	NiO (10/10)	NiO (20/10)	NiO (40/10)	NiO (80/10)
$V_{B}(V)$	840	4767	3095	3840	2543
$R_{ON} (m\Omega \text{ cm}^2)$	6.7	11.3	12.5	7.6	6.6
$V_{\rm B}^{2}/R_{\rm ON}~({\rm GW~cm}^{-2})$	0.11	2.01	0.77	1.95	0.98

TABLE I. Summary of conventional Ga₂O₃ and heterojunction NiO/Ga₂O₃ rectifiers. The thickness of the two NiO layers in nm is shown.



FIG. 6. Log plot of forward current densities and $R_{\rm ON}$ values from conventional Ga_2O_3 and double layer NiO/Ga_2O_3 heterojunction rectifiers with different NiO thicknesses.



FIG. 7. Compilation of Ron vs V_{B} of conventional and NiO/Ga_2O_3 heterojunction rectifiers reported in the literature.

and low on-resistance. Through design of the ultra-thin (20 nm) double-layer NiO structure, the V_B is substantially improved to 4.7 kV with an R_{on} of 11.3 m Ω cm² and a figure-of-merit (V_b^2/R_{on}) of 2 GW cm⁻². The high V_B is attributed to the structure of both the double-layer and the NiO extension to provide edge termination. From the TCAD simulation, the peak of the electric field is located at the edge of the diodes. Increasing the doping concentration of the NiO layer contacting Ni/Au can reduce the electric field at the edge of the

Ohmic contact. Simultaneously, the low doping concentration of the NiO contact with β -Ga₂O₃ can move the electric field maximum from the edge to the inside of devices. In addition, the extension guard ring can also reduce the electric field crowding. This work provides a desirable design strategy for NiO/Ga₂O₃ structures, leading to the highest breakdown voltage among all Ga₂O₃-based p–n diodes.

See the supplementary material for details on device structures and process parameters.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Jian-Sian Li: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Writing – original draft (equal). Chao-Ching Chiang: Conceptualization (equal); Data curation (equal); Writing – original draft (equal). Xinyi xia: Data curation (equal); Formal analysis (equal); Writing – original draft (equal). Timothy Yoo: Data curation (equal); Formal analysis (equal); Writing – original draft (equal). Fan Ren: Conceptualization (equal); Data curation (equal); Writing – original draft (equal); Writing – review and editing (equal). Honggyu Kim: Data curation (equal); Formal analysis (equal); Writing – original draft (equal). Stephen J. Pearton: Conceptualization (equal); Data curation (equal); Validation (equal); Writing – original draft (equal); Writing – review and editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material.

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