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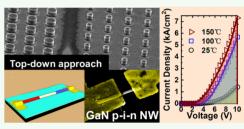


¹ GaN Single Nanowire p—i—n Diode for High-Temperature ² Operations

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4 ABSTRACT: III-Nitr	ide single nanowire (NW)-based 1	o—i—n diode wa	8 8 8 9 8 8 8 8 8 8

A ABSTRACT: In-Nitride single handwire (NW)-based p-1-n didde was s fabricated using a top-down etching method and its electrical and optoelectronic 6 characteristics were investigated from room temperature to high operation 7 temperatures up to 150 °C. The NW p-i-n didde exhibited good rectifying I-V8 properties at all measurement temperatures and the forward current could be 9 further enhanced when the temperature was increased. Simulation-based data 10 fitting revealed that the enhanced conduction was a result of increased carrier 11 concentration inside the NW, especially holes in the drift layer, as well as reduced 12 contact resistance. The reverse leakage current was kept low even at elevated



13 temperatures so that the UV (\sim 365 nm) responsivity remained high for a wide temperature range, suggesting the feasibility of NW 14 p-i-n diode for rectifying purposes and UV photon detection applications in high-temperature environments.

15 KEYWORDS: GaN, p-i-n diode, nanowires, high temperature, TCAD simulation, top-down method, UV detection

16 INTRODUCTION

17 The use of III-nitride (III-N) semiconductor materials for 18 various energy-efficient optoelectronic and electronic devices 19 has been extensively investigated due to III-N's wide energy 20 band gap, high critical electrical field, and good thermal 21 stability.¹⁻⁶ GaN p-i-n diode is a fundamental and important 22 device for a number of applications, such as rectifiers, 23 photodetectors (PDs), microwave switches, solar cells, and 24 so on.⁷⁻¹⁰ There has been tremendous progress in recent years 25 on thin film-based GaN p-i-n diodes on native GaN 26 substrates and foreign substrates.¹¹⁻¹³ Despite outstanding 27 device performance obtained for GaN p-i-n diodes grown on 28 native GaN substrates, bulk GaN substrates with low-defect 29 density are still expensive and only available in small sizes, 30 limiting their use for volume productions. GaN p-i-n diodes 31 grown on foreign substrates, such as Si and sapphire, show $_{32}$ dislocation density in the range of $10^6 - 10^9 / \text{cm}^2$, depending on 33 the lattice constant mismatch level, thin film thickness, and growth methods.^{8,14,15} Wide energy band gap III-N materials 34 35 are also promising for monitoring and detecting signals in high-36 temperature environments,^{16,17} such as furnaces, combustion 37 chambers, and so on. However, the defects may deteriorate the 38 device performance at high temperatures.

It is therefore imperative to synthesize and fabricate GaN p– 40 i–n devices out of nanostructures, $^{5,18-21}$ which are expected to 41 have low or zero dislocations inside by virtue of their nanoscale 42 dimension. $^{22-24}$ In addition, the one-dimension configuration 43 of nanowire (NW) p–i–n diode offers a direct and confined 44 carrier path for carrier transport inside the device under either 45 forward or reverse bias. The growth and characterization of GaN NW pn junctions ⁴⁶ have been extensively studied. GaN nanorod pn junctions ⁴⁷ grown on (111) Si substrates by plasma-assisted molecular ⁴⁸ beam epitaxy (PA-MBE) were transferred onto a SiO₂/Si ⁴⁹ substrate to investigate their photoresponse.^{5,25} In 2010, p–i– ₅₀ n junction GaN nanowire ensembles were synthesized and ₅₁ fabricated for visible–blind photodetectors.²⁶ The electrical ₅₂ characteristics of individual GaN p–n junction were measured ₅₃ by current–voltage (*I–V*) and electron beam induced current ⁵⁴ (EBIC), which demonstrated the presence of space charge ⁵⁵ limited current inside the NW.¹⁹ InN homogeneous p–i–n ⁵⁶ nanowires were grown on Si substrates and exhibited ⁵⁷ promising performance for solar cell applications.²⁷

An alternative way to fabricate GaN NW devices is the $_{59}$ "top-down" method, which starts from GaN layer structures $_{60}$ and utilizes etching tools to form nanoscale devices.²⁸⁻³⁰ A $_{61}$ number of device types have been demonstrated using this $_{62}$ scheme, including laser,^{31,32} light-emitting diode (LED),³³ and $_{63}$ transistor.^{29,34-38} There are a number of features for the NW $_{64}$ formed by the top-down approach. In addition to high $_{65}$ crystalline quality, the NW shares exactly the same epitaxial $_{66}$ materials as the starting thin film structure, presents control- $_{67}$

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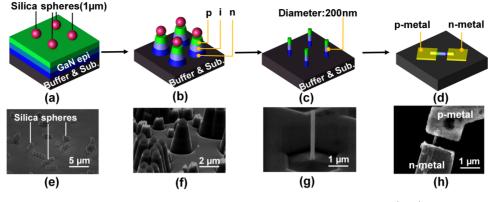


Figure 1. (a-d) Process flow of GaN single NW p-i-n diode using a top-down etching method. (e-h) Corresponding scanning electron microscopy (SEM) images after each fabrication step.

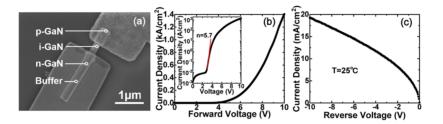


Figure 2. (a) SEM image of NW p-i-n diode. I-V characteristics of NW p-i-n diode under (b) forward and (c) reverse bias.

68 lable radial dimension by etching time, and is free of the 69 residual substance at the NW sidewall.^{29,39}

In this context, single GaN NW p-i-n diode has been r1 fabricated using a top-down etching scheme, starting from the GaN thin film grown on a sapphire substrate. With a radius of r3 100 nm and drift layer thickness of 500 nm, the GaN NW pr4 i-n diode showed good rectifying performance at 25 °C and r5 elevated temperature steps up to 150 °C. Technology r6 computer-aided design (TCAD) simulation tools were r7 employed to understand the carrier distribution and transport r8 behaviors inside the nanoscale device. The NW p-i-n diode r9 also showed high responsivity to UV light even at high 80 temperatures, showing its capability of working as a rectifier 81 and UV detector in harsh environments.

82 **EXPERIMENTS AND METHODS**

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83 Figure 1 illustrates the steps of fabricating single NW p-i-n diode 84 from GaN p-i-n epitaxial layers. The GaN p-i-n layers were grown 85 on a sapphire substrate using low-temperature grown GaN layer as a 86 seed layer and an unintentionally doped GaN layer as a buffer layer. 87 On top of the buffer layer, the p-i-n device structure was grown, 88 consisting of a 1 μ m-thick Si-doped n-GaN layer ($\sim n = 2 \times 10^{18}$ 89 cm⁻³), a 500 nm-thick undoped i-GaN layer, and a 500 nm-thick Mg-90 doped p-type GaN ($\sim p = 2 \times 10^{17}$ cm⁻³).

⁹¹ The NW fabrication process started from placing silica spheres (1 ⁹² μ m in diameter) on the GaN p–i–n thin film surface. Then, the GaN ⁹³ layers were etched by inductively coupled plasma etching (ICP) using ⁹⁴ the silica spheres as etching masks to form micron-sized GaN rods ⁹⁵ (Figure 1b), which would be further shrunk in an alkaline solution ⁹⁶ (AZ400K, 85 °C) to form vertical nanowires (Figure 1c). Upon wet-⁹⁷ etching in AZ400K, the nanowire with a desired radial dimension was ⁹⁸ obtained, and simultaneously, the damaged sidewall was eliminated ⁹⁹ from the nanowire, leaving a smooth surface for further nanowire ¹⁰⁰ harvest and metal deposition. Lastly, the vertical nanowires, which ¹⁰¹ had the same doping profile as the initial p–i–n film, were transferred ¹⁰² onto a SiO₂/Si substrate. After E-beam lithography, metal deposition, ¹⁰³ and lift-off, patterned metals were annealed to form contacts: 75/75 ¹⁰⁴ nm Ni/Au, 4 min 570 °C annealing in air for p-contact and 75/75 nm Ti/Au, 2 min 500 °C annealing in nitrogen for n-contact. Figure 1e-h 105 shows the corresponding SEM pictures for each key fabrication step. 106

Measurements of the p-i-n diode's I-V curves were performed at 107 room temperature and elevated temperatures up to 150 °C using the 108 voltage sweep mode from -10 to 10 V, while the substrate was at a 109 floating potential. For UV detection measurements, UV light sources 110 (365 nm) were employed to illuminate the NW p-i-n diode at 111 various power densities. A well-calibrated Si-based photodetector was 112 utilized to monitor the power density of UV light illuminated on the 113 NW diode so that the photoresponse could be further quantitatively 114 analyzed. 115

RESULTS AND DISCUSSION

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Figure 2a shows an image of the fabricated NW p-i-n diode, 117 f2 whose p-region and n-region are covered by its contact metal 118 while the i-region was exposed to outer ambience. The 119 nanowire used in this study was uniform in diameter and the 120 metal contacts covered the top half of the p-region and the n- 121 region. As shown in Figure 2b,c, the NW p-i-n diode shows 122 good rectifying I-V characteristics at room temperature. When 123 forward biased, the NW p-i-n diode showed a turn-on 124 voltage of 3.6 V at a current density of 1 A/cm^2 . The turn-on 125 voltage matches well with the energy band gap of GaN (3.4 126 eV). The forward current was exponentially increased as the 127 forward voltage, and the ideality factor was determined to be 128 5.7, which is larger than the number typically obtained for thin 129 film-based p-i-n diodes (2 to 3). The relatively large ideality 130 factor was correlated to the large contact resistivity that 131 occurred at the semiconductor/metal interface, especially at a 132 low bias range. In a separate experiment where the metal 133 contact was deposited onto a pure p-type nanowire, the 134 average specific contact resistivity was determined to be 135 around several $\Omega \cdot cm^2$ with bias smaller than 0.5 V. 136

Despite the large ideality factor at a low bias range, the 137 forward current density could reach 1.4 kA/cm² at a forward 138 bias of 10 V, and the corresponding specific on-resistance was 139 as small as 2.52 m Ω ·cm². The low differential on-resistance was 140

¹⁴¹ a result of carrier injection from the two terminals of the diode ¹⁴² as well as conductivity modulation. The reverse leakage current ¹⁴³ density of NW p-i-n diode was only 20 mA/cm² at a ¹⁴⁴ relatively large reverse bias of -10 V. The leakage current ¹⁴⁵ density was much smaller compared with some GaN NW p-¹⁴⁶ i-n diodes in the literature, ^{19,21,40,41} partly due to the absence ¹⁴⁷ of residual materials on the sidewall of the NW device using a ¹⁴⁸ top-down approach. The on/off current ratio (±10 V) was ¹⁴⁹ determined to be around 7 × 10⁴ at 25 °C.

150 The electrical characteristics of NW p-i-n diode at various 151 temperature steps are shown in Figure 3. Figure 3a,b illustrates

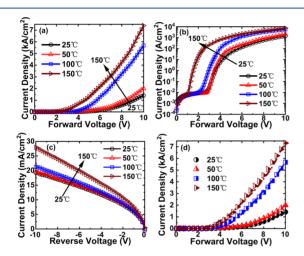


Figure 3. I-V characteristics of NW p-i-n diode at various temperatures in (a) linear scale and (b) logarithmic scale. (c) Leakage current density at various temperature steps. (d) Measured I-V characteristics (dash dot line) and corresponding data fitting curves (half-open symbols).

152 the current–voltage (I-V) characteristics of the NW diode at 153 various temperatures from 25 to 150 °C in linear scale and 154 logarithmic scale, respectively. As the temperature rose, an 155 increase in forward current was observed. Given the 1 A/cm² 156 current standard, the threshold voltage was gradually reduced 157 from 3.6 to 1.55 V, while the ideality factor was also 158 significantly improved from 5.7 at 25 °C to 2.3 at 150 °C. 159 The differential on-resistance of the NW was calculated to be 160 only 0.58 mΩ·cm² at 150 °C and the reverse leakage current 161 was still kept as low as 28 mA/cm² at high temperatures.

¹⁶² To understand NW p-i-n diode's temperature-dependent ¹⁶³ I-V behaviors, a simulation-based data fitting was performed ¹⁶⁴ using the TCAD simulation tool. Simulated I-V electrical ¹⁶⁵ characteristics of the NW diode at four different temperature ¹⁶⁶ steps are shown in Figure 3d, where all of the simulation results ¹⁶⁷ matched well with the measurement results. The GaN physical ¹⁶⁸ parameters used in this simulation such as electron affinity, ¹⁶⁹ carrier lifetime, carrier mobility,⁴² and specific contact ¹⁷⁰ resistance are summarized in Table 1^{42,43}

171 From the simulation-based I-V fitting, two mechanisms that 172 were responsible for the improved NW conduction were 173 revealed: enhanced carrier concentration in the drift region 174 and reduced contact resistance.

¹⁷⁵ Figure 4 illustrates the simulated carrier distribution along ¹⁷⁶ the NW *z*-axis at various temperatures at a fixed forward ¹⁷⁷ voltage of 3 V. At high temperatures, the electron-hole ¹⁷⁸ concentration product at equilibrium state would be ¹⁷⁹ considerably increased so that the minority carrier concen-¹⁸⁰ tration on either side of the junction would be augmented

Table 1. Parameters Used in Temperature-Dependent GaN NW Device I-V Simulations

parameters	quantity	unit	description
$E_{\rm g}$ (25 °C)	3.46	eV	direct band gap at 25 °C
affinity	4.1	eV	electron affinity
Con.resist (25 °C)	27	$m\Omega{\cdot}cm^2$	average contact resistivity at 25 °C
Con.resist (50 °C)	19.6	$m\Omega{\cdot}cm^2$	average contact resistivity at 50 $^\circ\mathrm{C}$
Con.resist (100 °C)	4.7	$m\Omega{\cdot}cm^2$	average contact resistivity at 100 $^\circ\mathrm{C}$
Con.resist (150 °C)	3	$m\Omega{\cdot}cm^2$	average contact resistivity at 150 $^\circ\mathrm{C}$
Mun1	100	$cm^2/V \cdot s$	arora low field mobility model
Mup1	12	$cm^2/V \cdot s$	parameter
Mun2	1200	$cm^2/V \cdot s$	
Mup2	145	$cm^2/V \cdot s$	
Alphan.arora	-1.5		
Alphap.arora	2		
Betan.arora	-1.5		
Betap.arora	-2.34		
Taun0 (25 °C)	0.7×10^{-9}	S	electron lifetime at 25 $^\circ\mathrm{C}$
Taup0 (25 °C)	2×10^{-9}	s	hole lifetime at 25 $^\circ \mathrm{C}$
Augn (25 $^{\circ}C$)	3×10^{-31}	cm ⁶ /s	Auger recombination parameter for electron at 25 °C
Augp (25 $^{\circ}C$)	3×10^{-31}	cm ⁶ /s	Auger recombination parameter for hole at 25 °C
EDB	0.017	eV	dopant activation energies for donor
EAD	0.160	eV	dopant activation energies for acceptor

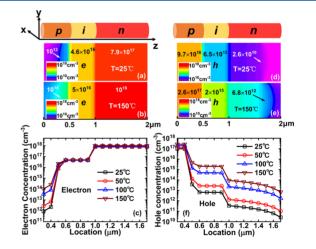


Figure 4. Extracted carrier information at forward bias of 3 V: electron concentration distribution along the axis of p-i-n diode at (a) 25 °C and (b) 150 °C. Hole concentration distribution along the axis of p-i-n diode at (d) 25 °C and (e) 150 °C. Extracted (c) electron and (f) hole concentration along the *z*-axis at various temperature steps.

according to the Shockley boundary conditions, as verified by 181 the simulation results of Figure 4c,f. The theoretical 182 calculations also suggested that the electron distribution in 183 the drift region typically remained the same, whereas the hole 184 concentration was greatly enhanced with increasing temper-185 atures. 186

Another factor that would help promote the forward current 187 was the reduction of contact resistance at higher temperatures. 188

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189 In a separate experiment, pure p-GaN and n-GaN nanowires
190 were also fabricated to measure the pure p-type and n-type
191 nanowire conductivity at various temperatures, as shown in
192 Figure 5. It was found that the conductivity was greatly

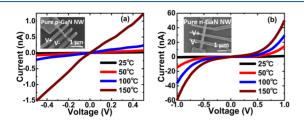


Figure 5. *I*–*V* characteristics of pure (a) p-GaN and (b) n-GaN NW at various temperature steps using two-terminal measurement methods.

193 improved as the temperature for both NWs was increased. Due 194 to the relatively larger activation energy of Mg dopant in p-195 GaN compared to that of the Si dopant in n-GaN, most of the 196 Si dopants have already been activated at room temperature, while a considerable portion of the Mg dopants can only be 197 198 activated at a higher temperature. With a higher hole concentration at a high temperature, a better metal/p-GaN 199 contact was thus obtained. For n-type GaN NW, the current 200 was increased sharply for V > 0.5 V, indicating a shallow barrier 201 202 for the metal/NW contact, leading to a nonideal ohmic 203 contact. The differential on-resistance was greatly reduced 204 from a few m $\Omega \cdot \text{cm}^2$ to several m $\Omega \cdot \text{cm}^2$ for V > 0.5 V. From the 205 simulation-based data fitting process, it was also found that a 206 reduction of average contact resistivity of the NW from 27 m Ω ·cm² at 25 °C to 3 m Ω ·cm² at 150 °C could well reproduce 2.07 the I-V characteristics. 208

Figure 6a shows the *I*–*V* characteristics of the NW diode in 210 dark condition and under UV light (λ = 365 nm) illumination.

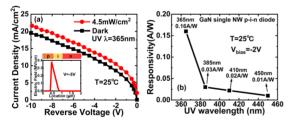


Figure 6. (a) Reverse current density of GaN single NW p-i-n diode in dark environment and under UV light (365 nm) illumination. (b) Wavelength-dependent responsivity of NW p-i-n diode at a reverse bias of -2 V.

211 An input UV light intensity of 4.5 mW/cm² on the NW 212 detector yielded a photocurrent density of 2.08 mA/cm², 213 corresponding to a responsivity of 160 mA/W at -10 V and 214 quantum efficiency of 54.1%. Further calculation revealed that 215 quite a uniform responsivity (150 ± 30 mA/W) was obtained 216 for the NW device under a wide range of bias up to -10 V, 217 measured under 4.5 mW/cm² 365 nm UV light illumination. 218 The measured responsivity of the NW photodiode was 219 much higher than that of the thin film p-i-n diode (15 mA/ 220 W) using the same epitaxial structure. This is because photons 221 from the UV sources could be directly absorbed by the drift 222 region of the NW device while there existed a significant 223 optical loss of photons in the path for thin film p-i-n diodes, 224 e.g., the light absorption in the p-GaN layer when used as a

front-illuminated PD. In addition to the absence of optical loss 225 in the optical path, another advantage of using nanowires as a 226 UV photodetector was that the electrical field inside the NW 227 under reverse bias was uniform along the radial direction (xy- 228 plane of Figure 4) and the peak electrical field was observed at 229 the p-i interface, which is designed to be exposed to UV light 230 for detection purpose. It should be noted that the surface 231 depletion effects, which have been observed for extremely 232 small nanowires,⁴⁴ have not been included in this study, partly 233 because the diameter was relatively large and the surface effects 234 have not been noticeably measured through substrate potential 235 alternation. The cut-off wavelength was found to be around 236 365 nm, which matches the direct energy band gap (3.4 eV) of 237 the GaN material. The NW PD also demonstrated a good 238 selectivity of UV (365 nm) to visible (450 nm) light, which 239 was measured to be about 16:1, much higher than that using 240 relatively narrower energy band gap materials. 241

Figure 7 shows the I-V characteristics of the fabricated GaN 242 f7 NW p-i-n diode in dark environment and under UV light 243

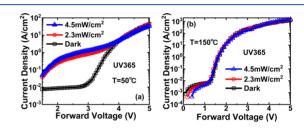


Figure 7. Forward I-V characteristics of NW diode in dark environment and under UV light (365 nm) illumination at (a) 50 °C and (b) 150 °C.

illumination at 50 and 150 °C. As shown in Figure 6a, at 50 244 °C, the current of the NW diode at a low bias range (2-3 V) 245 was greatly enhanced under UV illumination, which could be 246 attributed to extra carriers in the drift layer induced by the UV 247 light illumination. As a result, the threshold voltage of the NW 248 diode at 1 A/cm² was reduced from 3.65 V in dark 249 environment to 3.25 and 2.75 V under UV light illumination 250 of the power density of 2.3 and 4.5 mW/cm², respectively. 251

While at 150 °C, the forward characteristics for the NW 252 diode in dark and under UV light illumination tend to overlap 253 with each other for nearly the entire measurement bias range. 254 This could mean that the relatively weak UV illumination level 255 presented an insignificant effect on the current level and the 256 turn-on voltage, as the high temperature of 150 °C had already 257 boosted the carrier concentration and improved the contact 258 resistivity. 259

When the NW diode was reverse biased at 50 °C, the 260 responsivity of the diode (-5 V) was determined to be 212 261 mA/W with a 365 nm UV power density of 2.3 mW/cm². As 262 the temperature was elevated to 150 °C, both dark current and 263 photocurrent was increased, as summarized in Table 2. The 264 t2 responsivity and corresponding quantum efficiency of the NW 265 at -5 V was further enhanced up to 238 mA/W and 95.2%. 266 The elevated responsivity at high temperature mainly arises 267 from the increased density-of-states of the conduction band, 268 which thus promotes the transition rate of photon absorption 269 as well as photoresponse.⁴⁵ 270

CONCLUSIONS

Single nanowire-based III-nitride p-i-n diode was fabricated 272 using a top-down etching method. The fabricated nanowire 273

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Table 2. Measured Current Density in Dark and Under UV Illuminations at 50 and 150 $^\circ\mathrm{C}$

temperature (°C)	reverse voltage (V)	current in dark (mA/cm²)	current with UV 365 nm, 4.5 mW/cm ² (mA/cm ²)
50	-3	10.10	12.79
	-5	13.18	15.94
150	-3	13.31	16.42
	-5	17.84	20.94

274 featured a diameter of 200 nm and retained exactly the same 275 p-i-n structure along the axial direction as the initial GaN p-276 i-n epitaxial thin film. At 25 °C, the NW p-i-n diode 277 exhibited good rectifying I-V characteristics with a turn-on 278 voltage of 3.6 V at 1 A/cm² and leakage current as low as 7.4 279 pA at -10 V. The ideality factor was extracted as 5.7 and the 280 forward current density could reach 1.4 kA/cm² at 10 V. The 281 NW diode is also promising for high-temperature operations as 282 rectifiers and UV photodetectors. The forward conduction was 283 improved as the temperature was increased up to 150 °C, while 284 the reverse leakage current was only slightly increased due to 285 the wide energy band gap of the GaN materials. The NW 286 presented good UV (~365 nm) detection for a wide 287 temperature range that the responsivity was measured to be 288 around 160 and 238 mA/W at 25 and 150 °C, respectively. 289 The top-down etching approach and characteristics of GaN 290 NW p-i-n diode paved a promising path for its use in high-291 temperature and harsh environments.

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313 Author Contributions

314 [§]X. Zou and X. Zhang contributed equally to this work.

315 Notes

316 The authors declare no competing financial interest.

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