Highly uniform ultraviolet-A quantum-confined AlGaN nanowire LEDs on metal/silicon with a TaN interlayer

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Abstract: In this paper, we describe ultraviolet-A (UV-A) light-emitting diodes (LEDs) emitting at 325 nm based on a highly uniform structure of quantum-confined AlGaN quantum-disk nanowires (NWs). By incorporating a 20 nm TaN interlayer between a Ti pre-orienting layer and the silicon substrate, we eliminated the potential barrier for carrier injection and phonon transport, and inhibited the formation of interfacial silicide that led to device failure. Compared to previous reports on metal substrate, we achieved a 16 × reduction in root-mean-square (RMS) roughness, from 24 nm to 1.6 nm, for the samples with the Ti/TaN metal-bilayer, owing to the effective diffusion barrier characteristic of TaN. This was confirmed using energy dispersive X-ray spectroscopy (EDXS) and electron energy loss spectroscopy (EELS). We achieved a considerable increase in the injection current density (up to 90 A/cm²) compared to our previous studies, and an optical power of 1.9 μW for the 0.5 × 0.5 mm² NWs-LED. This work provides a feasible pathway for both a reliable and stable UV-A device operation at elevated current injection, and eventually towards low-cost production of UV devices, leveraging on the scalability of silicon substrates.

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References and links
1. M. A. Württele, T. Kolbe, M. Lipsz, A. Külb erg, M. Weyers, M. Kneissl, and M. Jekel, “Application of GaN-based ultraviolet-C light emitting diodes—UV LEDs—for water disinfection,” Water Res. 45(3), 1481–1489 (2011).
2. L. Krcmová, A. Stjernlof, S. Mehlen, P. C. Hauser, S. Abele, B. Paull, and M. Macka, “Deep-UV-LEDs in photometric detection: A 255 nm LED on-capillary detector in capillary electrophoresis,” Analyst (Lond.) 134(12), 2394–2396 (2009).
3. M. Kneissl, T. Kolbe, C. Chua, V. Kueller, N. Lobo, J. Stellmach, A. Knauer, H. Rodriguez, S. Einfeldt, and Z. Yang, “Advances in group III-nitride-based deep UV light-emitting diode technology,” Semicond. Sci. Technol. 26, 014036 (2010).
4. G. A. Shaw, A. M. Siegel, J. Model, and D. Greisokh, “Recent progress in short-range ultraviolet communication,” in Proc. of SPIE (2005), 215.
5. B. Janjua, H. Sun, C. Zhao, D. H. Anjum, D. Priante, A. A. Alhamoud, F. Wu, X. Li, A. M. Albadri, and A. Y. Alyamani, “Droop-free Al x Ga 1-x N/Al y Ga 1-y N quantum-disks-in-nanowires ultraviolet LED emitting at 337 nm on metal/silicon substrates,” Opt. Express 25, 1381–1390 (2017).
6. S. Zhao, A. T. Connie, M. H. Dashtjerdi, X. H. Kong, Q. Wang, M. Djavid, S. Sadaf, X. D. Liu, I. Shih, H. Guo, and Z. Mi, “Aluminum nitride nanowire light emitting diodes: Breaking the fundamental bottleneck of deep ultraviolet light sources,” Sci. Rep. 5, 8332 (2015).
7. S. Jahangir, M. Mandl, M. Strassburg, and P. Bhattacharya, “Molecular beam epitaxial growth and optical properties of red-emitting (λ = 650 nm) InGaN/GaN disks-in-nanowires on silicon,” Appl. Phys. Lett. 102, 071101 (2013).
24. Y.-H. Ra, R. Navamathavan, J.-H. Park, and C.-R. Lee, “High-quality uniaxial In_{x}Ga_{1-x}N/GaN Multiple Quantum Well (MQW) Nanowires (NWs) on Si(111) Grown by Metal-Organic Chemical Vapor Deposition (MOCVD) and Light-Emitting Diode (LED) Fabrication,” ACS Appl. Mater. Interfaces 5(9), 3355–3359 (2010).

25. S. Maeda, K. Tomioka, S. Hara, and J. Motohisa, “Fabrication and characterization of InP nanowire light-emitting diodes,” Jpn. J. Appl. Phys. 51(28), 248–258 (2002).

26. M. Wölz, C. Hauswald, T. Flissikowski, T. Gotschke, S. Fernández-Garrido, O. Brandt, H. T. Grahn, L. Geelhaar, and H. Riechert, “Epitaxial growth of GaN nanowires with high structural perfection on a metallic TiN film,” Nano Lett. 15(6), 3743–3747 (2015).

27. F. A. B. A. Alhamoud, X. Li, A. M. Albadri, A. Y. Alyamani, and B. S. Ooi, “Droop-Free, Reliable, and High-Power InGaN/GaN Nanowire Light-Emitting Diodes for Monolithic Metal-Optoelectronics,” Nano Lett. 16(7), 4616–4623 (2016).

28. B. J. May, A. G. Sarwar, and R. C. Myers, “Nanowire LEDs grown directly on flexible metal foil,” Appl. Phys. Lett. 108, 141103 (2016).

29. S. Q. Wang, S. Suthar, C. Hoeflich, and B. J. Burrow, “Diffusion barrier properties of TiW between Si and Cu,” J. Vac. Sci. Technol. B Microelectron. Nanometer Struct. Process. Meas. Phenom. 31(4), 456–458 (1980).

30. H. Ono, T. Nakano, and T. Ohta, “Diffusion barrier effects of transition metals for Cu/M/Si multilayers (M= Cr, Ti, Nb, MO, Ta, W),” Appl. Phys. Lett. 64, 1511–1513 (1994).

31. Y.-H. Ra, R. Navamathavan, J.-H. Park, and C.-R. Lee, “Formation of high-quality InGaN/GaN quantum-disk-in-nanowires on bulk-metal substrates for high-power light-emitters,” Nano Lett. 16(2), 1056–1063 (2016).

32. B. J. May, A. G. Sarwar, and R. C. Myers, “Fabrication of Nanowire Devices,” Small 14, 249–251 (1993).

33. I. Blech and E. Meieran, “Electromigration in thin Al films,” J. Appl. Phys. 40, 485 (1969).

34. C. S. Kang, H.-J. Cho, Y. Kim, R. Choi, K. Onishi, A. Shahriar, and R. C. Myers, “Semiconductor Nanowire Light-Emitting Diodes Grown on Metal: A Direction Toward Large-Scale Fabrication of Nanowire Devices,” Small 11(40), 5402–5408 (2015).

35. J. Tao, N. W. Cheung, and C. Hu, “Electromigration characteristics of copper interconnects,” IEEE Electron Device Lett. 14, 249–251 (1993).

36. S. A. Mirza, V. Fouquet, L. Pichon, M. Drouet, and A. Straboni, “Plasma assisted nitridation of Ti-6Al-4V,” Appl. Surf. Sci. 264, 342–349 (2010).

37. A. B. Bower and J. Mayer, “Growth kinetics observed in the formation of metal silicides on silicon,” Appl. Phys. Lett. 50, 342–349 (1982).

38. R. Bower and J. Mayer, “Growth kinetics observed in the formation of metal silicides on silicon,” Appl. Phys. Lett. 20, 359–361 (1972).

39. Y. L. Corcoran, A. H. King, N. de Lanerolle, and B. Kim, “Graz grain boundary diffusion and growth of titanium silicide layers on silicon,” J. Electron. Mater. 19, 1177–1183 (1990).

40. H. Kato and Y. Nakamura, “Solid state reactions in titanium thin films on silicon,” Thin Solid Films 34, 135–138 (1976).

41. S. Herd, K. Tu, and K. Ahn, “Formation of an amorphous Rh-Si alloy by interfacial reaction between amorphous Si and crystalline Rh thin films,” Appl. Phys. Lett. 42, 597–599 (1983).

42. W. Lur and L. Chen, “Growth kinetics of amorphous interlayer formed by interdiffusion of polycrystalline Ti thin-film and single-crystal silicon,” Appl. Phys. Lett. 54, 1217–1219 (1989).

43. A. Pierret, C. Bougerol, M. d. Hertog, B. Gayral, M. Kociak, H. Renevier, and B. Daudin, “Structural and optical properties of Alx Ga1–xN nanowires,” physica status solidi (RRL)- Rapid Research Letters 7, 868–873 (2013).
1. Introduction

AlGaN layered structures generating UV have been used in devices for bacterial disinfection [1], chemical agent detection [2], UV-curing [3], communications [4], and lighting [5] as they are composition-, and therefore wavelength-tunable, mercury-free, and have long term stability. However, the current technology still suffers from inadequate light extraction efficiency, piezoelectric polarization, threading dislocations, and low wall-plug efficiency, thus hindering the wide-spread utilization of these devices.

Compared to the matured planar quantum-well-based technology, light-emitting diodes (LEDs) based on group III-nitride nanowires (NWs) have been studied in recent years as they offer dislocation-free crystals, feasibility of reduced polarization field devices and growth on scalable silicon substrates for cost effectiveness as well as potential III-V/silicon integration. Devices operating in the UV and visible range with high internal quantum efficiency (IQE) and almost without efficiency droop have been demonstrated. Mi et al., employing N-polar AlGaN NWs on Si, reported an 80% IQE (assuming nearly unity IQE at 20 K), where the polarization field is anti-parallel to the intrinsic electric field and favors carrier transport [6].

In the visible range, Jahangir et al. demonstrated 50% IQE for a device emitting at a peak wavelength of 650 nm by post-passivating the NWs on Si with SiN [7].

Recently, we have demonstrated AlGaN-based NWs on Ti/Si-substrate that emit at 337 nm; this exploits the natural formation of conductive TiN, in preference to an insulating SiNx layer [5]. However, the high temperatures usually employed in molecular beam epitaxy (MBE) processes cause interdiffusion through the metal/Si interface and can lead to a reduction in the Ti metal thickness, depending on process duration and temperature. These conditions can also result in a rough surface and subsequent non-uniform, misoriented, or mixed-orientation growth of NWs. In fact, Myers’ group reported that the high thermal mismatch between Ti and Si (thermal expansion coefficients of $8.4 - 8.6 \times 10^{-6}$ K$^{-1}$ and $2.6 - 3.3 \times 10^{-6}$ K$^{-1}$, respectively), as well as high-temperature oxide desorption during the MBE process, cause delamination of the Ti thin-film from the Si substrate [14]. Despite the advantage of incorporating Ti metal, which leads to the formation of TiN ohmic contacts and facilitates lateral and vertical heat and current spreading, we found that Ti/Si interdiffusion and the resultant surface roughness on the metal/silicon eventually results in delamination and catastrophic device failure at high injection current or elevated temperature.

In this study, we address the interdiffusion and related roughness issues to permit large-scale production of NW-LEDs using well-established silicon foundry processes. One solution is to place a diffusion barrier layer to limit interdiffusion. Al and Cu are used for contacts and interconnect materials due to their low resistivity in integrated circuits [15, 16]; diffusion barriers for Cu metallization such as TiN [17], Ta [18], Ti-W [19], and TaN have been investigated to prevent interdiffusion and improve device reliability [20]. A transition metal
nitride, such as TaN, is desirable for having a low resistivity (in the range 0.130–150 mΩ·cm, depending on the N flow rate) [21], a high melting point (>3000 °C), and compatibility with high temperature MBE growth processes (>800 °C). In a similar manner, this investigation resolves two key technology bottlenecks in enabling practical utilization of silicon substrate for quantum-confined AlGaN nanowires devices, thus allowing reliable and facile fabrication of reduced polarization field UV-LED on scalable substrate. The investigation involves the design of the first interfacial metal layer eliminating the potential barrier for carrier injection and phonon transport. This is followed by the second interfacial metal layer to inhibit the formation of interfacial silicide that leads to device failure, such as device delamination, as encountered by other research groups neither utilising metal nor metal-bilayer. Hence our design of metal bilayer, as introduced in this first report, and the evidence of interfacial integrity (electron-microscopy data) as well as device performance, serve to enlighten and educate researcher in the field of compact, mercury-free UV-light source, and wide-bandgap materials engineering in general. The study aims to advance the nanowires research towards practical demonstration, beyond basic research, since the seminal studies and interest in the nanostructure device.

We deposited a pre-orienting Ti layer on a ~20 nm TaN diffusion barrier to exploit the integrity of Ti; this allows subsequent facile fabrication without the need for a planarization layer, such as parylene [22], BCB [23], polyimide [24], or spin-on glass [25], which prevent short-circuits when metal-contacts are deposited. The resulting Ti/TaN/Si template has a RMS roughness of ~1.6 nm, compared to ~24 nm for a Ti/Si template without a TaN barrier insertion. The Ti/TaN/Si interfaces were clearly distinguishable in transmission electron microscope imaging, Electron Dispersive X-ray spectroscopy (EDXS) and Electron Energy Loss spectroscopy (EELS), indicating insignificant interdiffusion. The substrate flatness and smoothness achieved are also essential for growth of NWs and device fabrication. Using this approach to achieve scalable and reliable high electrical injection devices, we demonstrated UV-A LEDs based on AlGaN quantum-disks (QDisks) in NWs with output power of 1.9 μW, and current injection up to 90 A/cm². The electroluminescence (EL) spectrum showed fixed peak emission at 325 nm for a wide range of driven currents with a full-width at half-maximum (FWHM) of 17 nm. Our approach of implementing metal-bilayer for reliable device operation allows researchers in the field to continue to explore into and unleash the potential of nanowires AlGaN devices. Indeed, the NWs device technology is at its infancy, compared with the already matured planar nitrides. Therefore this constitutes an important research effort in advancing the AlGaN nanowires devices.

2. Experimental section

In this experiment, a ~20 nm TaN diffusion barrier was deposited on a 20% HF-cleaned 0.25 mm phosphorus-doped <100> Si substrate (10⁻¹¹ Ω·cm) using atomic layer deposition (ALD) at 300 °C, followed by an ~80 nm Ti layer deposited by an e-beam evaporator. Ta precursor was purged with 200 sccm Ar and H₂ plasma (50 sccm). The Ti/TaN/Si template was then outgassed in the MBE load lock at 200 °C for 1 h followed by outgassing in the buffer chamber at 600 °C for 2 h, to remove moisture and molecular adsorption for subsequent growth.

The n-GaN seeds were initiated at a substrate temperature of 485 °C for 10 min to reduce adatom desorption and increase the nucleation probability. The Ga beam equivalent pressure (BEP) was 6.2 × 10⁻⁸ Torr, the Si effusion cell was kept at 1165 °C, and the high-brightness nitrogen plasma was sustained using 350 W RF power and 1 sccm flow rate. A second nucleation step at 585 °C for 20 min was used to improve the crystal quality. In total, ~85 nm of n-GaN was grown, and verified using transmission electron microscopy (TEM). The temperature was then raised to 640 °C to grow a 50 nm n-AlGaN bottom barrier-layer. We estimated the nominal Al composition from the ratio of the Al-BEP compared to that of Ga. The active region is composed of 10 stacked repetitions of alternating AlₓGa₁₋ₓN (QDisks)
(Al and Ga BEP of $0.75 \times 10^{-8}$ and $4.5 \times 10^{-8}$ Torr) and Al$_x$Ga$_{1-x}$N quantum barriers (QBs) (Al and Ga BEP of $1.5 \times 10^{-8}$ and $3 \times 10^{-8}$ Torr) (where $x < y$) with thicknesses of 3 and 4 nm, respectively, also grown at 640 °C. The ~50 nm p-contact AlGaN cap layer was then grown at 620 °C for 60 min at Al and Ga BEP values of $1.5 \times 10^{-8}$ and $2 \times 10^{-8}$ Torr, respectively, while the Mg cell temperature was kept at 440 °C with the same nitrogen plasma conditions. An additional highly doped layer of AlGaN, p'-AlGaN, was grown atop the p-AlGaN by increasing the Mg cell temperature to 450 °C and reducing the growth temperature to 580 °C, resulting in a p'-AlGaN/p-AlGaN combined thickness of ~20 nm. To be noted is the lack of p-GaN contact layer which can diminish the UV absorbance and increase the light extraction.

The UVA NWs-LEDs were fabricated using standard UV contact-lithography techniques. The sample was dipped in 20% HF for native oxide removal immediately before Ni/Au (5 nm/5 nm) blanket-evaporation and 1 min at 550 °C RTP step. Further evaporation of Ni/Au (10 nm/400 nm) was carried out to define contact-fingers and probe-pads using photoresist and UV contact lithography, using the metal-lift-off technique. Finally, the Si back-surface was etched away by 200 nm using inductively coupled plasma reactive-ion etching (ICP RIE) (SF$_6$: 15 sccm; O$_2$: 4 sccm; RF power: 50 W; ICP power: 500 W; pressure: 10 mTorr) in preparation for depositing Ti/Au (10 nm/150 nm) n-contacts.

For evaluating surface morphology, atomic force microscope (AFM) measurements were taken using an Agilent 5400 SPM with a scan range of 90 μm × 90 μm × 8 μm and a vertical noise of 0.016 nm. This is then correlated with a structural and compositional characterization by TEM combined with EELS and EDXS. For this study we used Titan Themis Z TEM from FEI Co (currently Thermo Fisher, USA) equipped with Gatan Quantum 966 imaging filter and Super-X EDXS detector. Microscope was operated at 200 kV in scanning (STEM) mode. High resolution scanning electron microscopy (SEM) images were taken using FEI Nova Nano 630.

A 266-nm pulsed laser (Teem Photonics SNU-20F-100; 10 mW average power, 0.7 kW peak power, 0.6 ns pulse width, 19 kHz repetition rate) mounted in a reflective configuration was used for both low- and room-temperature photoluminescence (PL) measurements. The light emission was collected through a 15 × objective lens (Thorlabs LMU-15X-UVB; focal length 13 mm and numerical aperture (NA) of 0.32, with anti-reflection (AR) coating for the 240-360 nm wavelength range), a 50:50 beam-splitter (Thorlabs BSW19, AR coated for 250-450 nm) to distribute the light to the focusing lenses of a viewing camera, and a monochromator (Andor Shamrock-750) equipped with a Si-based CCD (Andor iDus DU420A-OE). For the PL measurements, the 266-nm laser excitation was filtered using an ultra-steep long pass edge-filter (Semrock LP02-266RU-25). This setup was also used for the electroluminescence (EL) measurements. Light output – current – voltage (L-I-V) measurements were performed using a direct-current (DC) source meter (Keithley 2400) and a silicon photodetector with a power meter (Newport 818-UV and 1936-C, respectively). The sheet resistance was measured using a four-point probe system (MDC CMT-SR2000N) having a measuring range from 1 mΩ/□ to 2 MΩ/□ and an accuracy of ± 0.5% (at 23°C).
3. Results and discussion

Fig. 1. Morphological and structural characterization of template substrates developed in this investigation: AFM analysis of (a) Ti/Si (Ti on Si substrate) and (b) Ti/TaN/Si (Ti on TaN/Si). (c) Comparative statistical analysis of RMS roughness for (a) and (b). (d) STEM and EELS maps of the Ti/TaN/Si template substrate prior to growth of NWs, showing a sharp interface and distinct layer-structure, indicating the absence of Ti-Si interdiffusion.

One of the main challenges of growing NWs on novel substrates is to begin with a flat surface on which to obtain highly uniform NWs. This is especially significant for the fabrication of devices. We analyzed the surface of our substrates using AFM on a 36 μm² area. Figure 1 (a-b) shows the surface roughness comparison between the Ti/Si and Ti/TaN/Si template substrates. An average RMS roughness of 24 nm is seen for the Ti/Si, whereas Ti/TaN/Si shows 1.6 nm, a reduction of more than 95%. Figure 1(c) shows a statistical analysis of AFM-determined roughness in different locations on the samples to confirm the homogeneity of the surface. No large differences are observed, meaning that the deposition of the TaN and Ti layers is uniform throughout the samples.

To confirm the presence of the TaN barrier layer and the surface roughness, we analyzed the samples by STEM and EELS. Figure 1(d) depicts a zoomed-in image of the Ti/TaN/Si template substrate used for AFM measurement, prior to NW growth and after buffer chamber outgassing, and the elemental mapping of each layer. It is clear that no significant reaction between the layers is observed and the Ti surface roughness is qualitatively correlated with that of the AFM results. This is due to the absence of TiSi, and, consequently, of tensile stress [26].
Fig. 2. (a-b) Comparison of SEM micrographs for AlGaN NWs LEDs structure showing the rough surface and the height inhomogeneity for NWs grown on (a) Ti/Si, and the improvement for NWs on (b) Ti/TaN/Si. (c) Cross section dark-field STEM (Z-contrast) image of the Ti/TaN/Si sample (the red dash-line shows the boundary of a single nanowire). (d-g) EDXS elemental mapping of the Ti/TaN/Si sample for (d) Si, (e) Ta, (f) N, and (g) Ti, Ga, and Al. (h) EELS elemental mapping of Ti/Si template substrate showing a clear interdiffusion with 20% Ti (~15 nm) remaining after outgassing at 600 °C, and subsequent growth of NWs at 640 °C.

The structural characteristics of the Ti/Si and Ti/TaN/Si substrates after NWs growth were analyzed using SEM and TEM. Figure 2(a-b) shows a SEM cross section of the NWs grown on the two substrates, with a length of 300-350 nm and diameter of 90-100 nm. The NWs show an inverse tapered shape, thinner at the bottom and larger at the top, due to the growth temperature gradient and lateral growth preference. The NWs grown on the Ti/TaN/Si template substrate show a greater flatness compared to those grown on Ti/Si, as well as better height homogeneity. We also observed a spontaneous coalescence of the top p-AlGaN layer, resulting from the temperature dependence of the natural lateral growth rate of p-doped GaN. The average density was estimated to be $8 \times 10^9$ cm$^{-2}$.

Figure 2(c) shows the STEM image of the full structure used for the EDXS elemental mapping measurement (Fig. 2(d-g)). A slight Si interdiffusion is noticed extending 40 nm above the substrate, into the TaN barrier (Fig. 2(d)). However, beyond that, Si is not detected, indicating that the TaN prevented the layers from corrupting each other and allowed the Ti to form a flat surface for the NWs' growth. The dark band that appears above the TaN interlayer is due to a lack of materials (small crack) due to Focus Ion Beam (FIB) sample preparation. Further experiments with 5 nm and 10 nm TaN layers were also conducted for diffusion barrier optimization (not reported in this manuscript) but such thicknesses were not enough to impede the interdiffusion. In Fig. 2(e), we show a Ta elemental map. Other than the strong Ta signal from the interlayer, faint signal was also observed in the nanowire section. This is due to the presence of Cu signal originated from the FIB grid, which overlaps with the Ta signal in EDXS. Figure 2(f) shows the nitrogen EDXS map. Under plasma irradiation, N diffuses throughout Ti to form primarily a conductive $\delta$-TiN layer at the surface, due to the small plasma influence on the deep N diffusion process [27]. Fig. 2(h) shows the EELS elemental mapping of the Ti/Si substrate after outgassing in the MBE buffer chamber and subsequent NWs growth at the same temperatures as the Ti/TaN/Si sample. As expected from the parabolic trend of the titanium silicide growth rate [28], 80% of the Ti is transformed into...
TiSix. The high diffusivity of Si in Ti is reduced as the silicide grain size increases. In fact, the silicon flux through Ti grain boundaries depends on the silicide grain radius and the diffusion width of the grain [29]. As reported by Kato, the TiSi2 phase dominates above 600 °C [30]. As the NWs growth took place at 640 °C, we can assume we obtained the same phase. Moreover, previous reports show the presence of an amorphous interlayer between the metal and the semiconductors [31], and more specifically, between the Ti and crystalline silicon, after annealing at 600 °C [32]. However, such a layer was not found in our study. In addition, the Ti surface appears to be rough, most probably due to a tensile stress of approximately \((1-2) \times 10^{10} \text{ dyn/cm}^2\) (for a 100 nm Ti layer), which builds up in the film at high temperatures with increasing TiSi2 growth [26].

Next, we examined the evolution of PL characteristics for assessment of AlGaN-based nanowires material quality when they are grown on the metal-bilayer. Figure 3(a) shows the temperature-dependent PL (TDPL) from 10 to 300 K. A strong peak appears at ~320 nm due to the QDisks recombination process and a second peak emerges at 288 nm, resulting from the short diffusion length of excess carriers at low temperatures that gives rise to radiative recombination in the quantum barrier. When deconvoluted into two Gaussian curves (e.g. inset in Fig. 3(a)), it is noted that the FWHM values for the QDisks-related Gaussian component are almost constant \((18.1 \pm 0.2 \text{ nm})\) versus temperature (Fig. 3(b), blue curve), signifying negligible inhomogeneous and homogeneous broadening. The FWHM values are close to that of our previous reports \((-15 \text{ nm})\) [5, 8], and thus material quality is adequately preserved when metal bilayer is implemented. The relatively small value of 18.1 nm indicates insignificant fluctuations in composition, and also that there is quantum confinement effect. Unlike in InGaN-based structures, where indium compositional fluctuation dominates [33], which results in large emission spectrum broadening, AlGaN materials are less prone to temperature variations [34], hence showing smaller composition modulation and in turn narrower PL FWHM [35]. On the other hand, the QDisks emission peak changes from 317 nm (3.912 eV) at a temperature of 10 K to 321 nm (3.863 eV) at room temperature, as predicted by the Varshni empirical equation.
Fig. 4. AlGaN NWs LED characterization: (a) linear and semilog plots of current-voltage characteristics showing ~8-V turn-on voltage; and (b) power-voltage characteristics showing up to 1.9 $\mu$W optical power. Inset shows AlGaN NWs LED structure. (c) Electroluminescence spectra at different injection currents (from 10 mA to 110 mA), showing a peak wavelength of 325 nm. Inset depicts the shift in peak wavelength (Peak $\lambda$) and FWHM with increasing current (I). (d) Plot of relative external quantum efficiency (relative EQE, or $\eta_{ext} = (P/h\nu) / (\frac{I}{e})$) vs. injection current.

Figure 4(a) depicts the I-V characteristics of the UV AlGaN-NW LEDs, with both linear and logarithm scales used for the current density to confirm the diode behavior. The turn-on resistance was measured to be 14.3 $\Omega$ by linearly extrapolating the I-V exponential region (red dashed line). We were able to inject current at a density up to 90 A/cm$^2$, indicating that the Ti/TaN contact layer is stable. As the work function of TaN is in the range 3.4–4.1 eV [21] and the electron affinity of silicon is ~4.29 eV [36], a TaN-Si junction forms an ohmic contact, improving the electrical conductivity. We measured the sheet resistance for TaN (20 nm) on Si (TaN/Si) before and after annealing (640 °C for 1 min in vacuum), Ti (80 nm) on Si (Ti/Si), and for Ti on TaN/Si after outgassing (in the MBE load lock at 200 °C and the buffer chamber at 600 °C); the results are presented in Table 1. The small sheet resistance decrease (18.5%) for the TaN/Si sample upon annealing can be neglected in comparison to the range of reported Ti/Si values (20–25 $\Omega$/$\square$ at RT) for different annealing temperatures [26, 37]. However, the small value of 2.93 $\Omega$/$\square$ for outgassed Ti/TaN/Si, in comparison to Ti/Si (25.89 $\Omega$/$\square$), cannot result from a TiSi$_2$ layer; Fig. 1(d) shows the TaN barrier that prevents the silicide formation. On the other hand, the low sheet resistance may be related to the underlying highly conductive TaN layer in parallel to the Ti.
Table 1. Sheet resistance of different layer structures.

| Layer Structure               | Sheet Resistance (Ω/□) |
|-------------------------------|------------------------|
| Silicon substrate             | 138.02 ± 0.39          |
| TaN/Si-substrate              | 1.85 ± 0.20            |
| Annealed TaN/Si-substrate     | 1.51 ± 0.02            |
| Ti/Si-substrate               | 25.89 ± 0.15           |
| Outgassed Ti/TaN/Si-substrate | 2.93 ± 0.03            |

A large bandgap p-AlGaN contact-cap layer was grown instead of p-GaN, giving a turn-on voltage of ~8 V, which is comparable to our previously reported value [5]. An output power of 1.9 μW at 12 V was also achieved as depicted in Fig. 4(b) for the NWs LED layer-structure shown in the inset. This is an improvement over our previous devices, in part because of the higher light extraction efficiency from using a non-absorbing (at 325-nm wavelength) p-AlGaN layer. In addition, the present device has a larger number of NWs being injected, as a result of the improved NW-height homogeneity when grown on the Ti/TaN/Si template. Further, we underestimate the measured power as the microscope objective does not collect the full solid angle of the Lambertian radiation pattern. It is notable that saturation or thermal roll-over in the light output power is not observed up to 90 A/cm² (12 V); this signifies that operation at high injection current density is feasible with the use of a Ti/TaN/Si template, with reliable process and device performance.

For room temperature EL measurement, current was varied from 10 to 110 mA as shown in Fig. 4(c), with peak emission at 325 nm when injected with 110 mA. This is close to the RT PL at 320 nm, confirming that QDisks are responsible for emission from the active region. The inset shows that peak emission wavelength is independent of injection current density. This is explained by the reduction in the quantum-confined Stark effect resulting from a lower piezoelectric polarization field-related strain. In fact, unlike those planar structures that are highly affected by polarization fields [38], NWs are strain-relieved structures, hence the blue shift that is typically observed with change in injection current is insignificant. The FWHM initially decreases rapidly with injection current, until ~30 mA when the trend reverses and inhomogeneous broadening gradually increases it.

The relative external quantum efficiency (EQE) was calculated with the formula depicted in Fig. 4(d) where \( P \) is the optical power obtained in Fig. 4(b), \( h\nu \) is the photon energy (Fig. 4(c)), \( I \) is the injection current and \( e \) is the electron charge. We observed that the EQE rapidly increases with the injected current and reaches a plateau beyond 50 A/cm².

We also tested the stability of the device shown in the inset in Fig. 5 over approximately 6 h with an injection current density of 72 A/cm² (Fig. 5), noting that the device is still functional beyond the 6-hour test period. The behavior shows one of the typical trend when device is subjected to an excessive burn-in cycle. Although the power rapidly decreases in the first hour, it then stabilizes without showing device failure at the high injection current, indicating that the NWs-based UV device can sustain a high injection current for a prolonged period of time.
4. Summary

In conclusion, UV-A LEDs based on an AlGaN NWs structure were demonstrated on metal-bilayer/silicon for reliable operation at high injection current. By implementing a TaN diffusion barrier, we significantly reduced the formation of TiSi$_2$, as confirmed by EDXS and EELS imaging, and the roughness resulting from the high-temperature MBE process, thereby preserving the smoothness of a Ti pre-orienting layer. As a result, RMS roughness of 1.6 nm was achieved on a Ti/TaN/Si template as compared to 26 nm on a Ti/Si template. This approach enables the growth of uniform nanowires with improved electrical efficiency and reliability. The fabricated NW-LED shows 1.9 μW light output power with an electroluminescence peak at 325 nm under DC operation, tolerating a high injection current density up to 90 A/cm$^2$. The improved process contributed to the progress in diode-based UV-A LED technology, potentially opening a pathway towards eventual low-cost UV devices leveraging on scalable silicon substrate technology.

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