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III-Nitride Based Narrow Band Far-UVC LEDs for Airborne and Surface Disinfection

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Narrow-band far-ultraviolet C ($\lambda = 200\text{-}230$ nm) light-emitting diodes (far-UVC LEDs) are strongly detrimental to airborne pathogen like bacteria and viruses while minimally invasive to human health so they can be used as a disinfectant to suppress the outbreak of infectious diseases with minimum safety concerns. Herein, we investigate a design of AlGaIn/AlN nanowire structure in combination with a bandpass filter for a narrow band far-UVC LED at 222 nm center wavelength. The LED achieves an ultra-narrow full width at half maximum (FWHM) of ~ 12 nm after introducing a metal-dielectric Fabry-Perot optical bandpass interference filter with three periods of Al/MgF₂/Al layers. The electrical and optical properties of the nanowire LEDs show the high performances with an internal quantum efficiency (IQE) up to 80% and the maximum power exceeding 10 mW at a current injection of 60 mA. This narrow-band far-UVC LED is a promising candidate for airborne and surface disinfection in occupied spaces to prevent the spread of contagious diseases.

Introduction

III-nitride compounds have gained momentum in research and development for UVC LEDs owing to their wide direct band gaps which cover the nearly entire ultraviolet regime ($\sim 200\text{-}365$ nm). However, the high-quality Al-rich epitaxial layers often have a high density of threading dislocations (over $10^8/\text{cm}^2$). Especially far-UVC LEDs, which require a very high Al amount in AlGaIn for wavelengths, are very limited in their quantum efficiency. Other challenges also arise from inefficient Mg-doped *p*-type activation, high spontaneous polarization, and piezoelectric polarization induced by lattice mismatch between AlN and GaN. In this context, nanowire structures have emerged as a promising candidate for highly efficient far-UVC LEDs. Nanowire structures have several advantages over their counterpart planar structures. First, since a nanowire can release effectively the induced strain energy into its sidewall, nanowire epitaxial growth can attain a low level of threading dislocations and total polarization [1, 2], thus minimizing defects and quantum confined Stark effects (QCSE) [3], compared to the thin film UV LEDs. Second, due to the high surface area-to-volume ratio, the diffusion of atomic Mg acceptors at the nanowire's surface could easily happen, beneficial for a highly doping concentration in AlGaIn/AlN nanowires [4]. Third, nanowire structure LEDs outperforms their counterpart thin-film LEDs in terms of the light extraction efficiency (LEE) [5]. Finally, high quality crystalline nanowires could be realized on a wide variety of substrates including cost-beneficial Si wafers [6].

Airborne and surface disinfection are one of the most promising for UV LEDs among their various applications in water/air purification, UV curing, phototherapy, biology, and neuroscience [7-9]. In airborne and surface disinfection in occupied spaces, far-UVC

LEDs at 222 nm is preferable, because photons in this wavelength are almost absorbed by the human's dead skin cell layer, thereby being surely harmless to humans [10]. In this work, 222 nm far UVC nanowire LEDs are investigated with an advanced numerical device simulation method to the nanowire LED structure, simple enough for easily epitaxial growth in an empirical research. Advanced Physical Models of Semiconductor Devices (APSYS) software is used to study the performance of the UV nanowire LEDs in this study. The far-UVC LEDs consist of a single quantum well of $\text{Al}_{0.855}\text{Ga}_{0.145}\text{N}$ active region. APSYS is a commercial computational simulator which has been widely used in LED design and validation. Its solvers utilize the self-consistent solutions of many quantum mechanics equations including Schrodinger, Poisson, carrier transport, current continuity, quantum mechanical wave, and photon rate equations with suitable boundary conditions. Simulation results yield necessary parameters for the evaluation of the LED through its energy band diagram, internal quantum efficiency, current-voltage characteristic, and output power, etc.

For airborne surface disinfection, a narrow spectrum is highly desirable to precisely trigger biological events for avoiding harmful impact on humans [11]. Therefore, far-UVC LEDs are an ideal disinfectant for occupied spaces when photons in these wavelengths do not penetrate deep into the living cells in the dermis and epidermis layers [12-14]. Generally, UVC LEDs usually possess a FWHM of >25 nm. Therefore, to produce a narrow spectrum, an integrated bandpass interference filter is necessary to achieve narrow-band far-UVC LEDs. A filter is designed from a Fabry-Perot structure having the stack of Aluminum/Magnesium Fluoride layers. A starting structure includes three periods of Al/MgF₂/Al layers. OpenFilter, an open-source software, is used to optimize the bandpass filter by adjusting the thickness of each layer. The maximum transmission is achieved over 50% with a FWHM of ~ 12 nm. With two simulation tools, APSYS and OpenFilters, a simple effective AlGaN/AlN nanowire structure has been demonstrated for high performance narrow band 222-nm far-UVC LEDs, thus ideal for surface disinfection applications.

Device Structure and Simulation Parameters

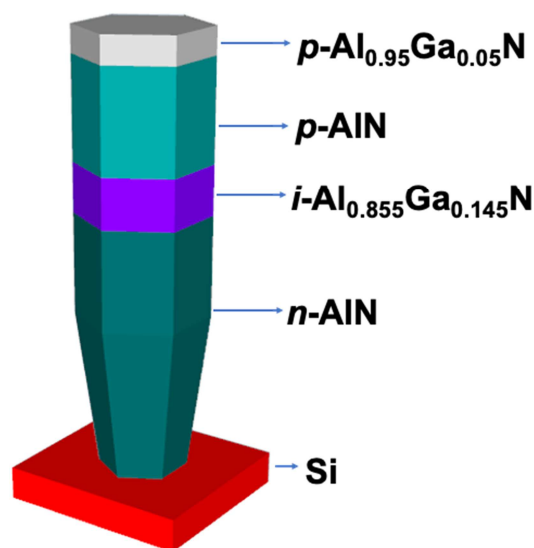


Figure 1. The schematic structure of the AlGaN/AlN nanowire based far-UVC LED.

Because the growth of a high crystalline quality of Al-rich AlGaN LEDs with multi-quantum wells is difficult, so a simple *n-i-p* LED structure with a high performance is expected to benefit for UV LEDs. Therefore, in this study, the advanced numerical device simulation with APSYS software is applied to investigate the performance of the *n-i-p* AlN/AlGaN nanowire UV LED at 222 nm. The schematic of an LED nanowire consists of 300 nm *n*-AlN/ 40 nm *i*-AlGaN/ 100 nm *p*-AlN/ 20 nm *p*-Al_{0.95}Ga_{0.05}N, which is considered to be grown on a (111) silicon wafer as shown in Figure 1. The *n*-AlN layer is the Si-doped layer ($n_D = 2 \times 10^{18} \text{ cm}^{-3}$) and the Si energy activation is set at 15 meV [15]. The active region is an intrinsic Al_{0.855}Ga_{0.145}N of 40 nm. The *p*-region is a Mg doped *p*-AlN ($N_A = 2 \times 10^{18} \text{ cm}^{-3}$) with the thickness of 100 nm. Finally, a thin *p*-Al_{0.95}Ga_{0.05}N ($N_A = 10^{20} \text{ cm}^{-3}$) is employed on the top of the nanowire to form an ohmic contact. The Mg activation energy for *p*-AlN and *p*-Al_{0.95}Ga_{0.05}N is set at 630 meV and 608.5 meV, respectively [15]. To obtain 222 nm emission, 85.5% of AlN composition in Al_xGa_{1-x}N is calculated from the formula: $E_{AlxGa1-xN} = xE_{AlN} + (1-x)E_{GaN} - bx(1-x)$, where $b = 1$ is chosen [16]. The radiative recombination coefficient is set at $2.13 \times 10^{-11} \text{ cm}^3/\text{s}$, Auger recombination coefficient $2.88 \times 10^{-30} \text{ cm}^6/\text{s}$ and the Shockley-Read-Hall (SRH) recombination lifetime 15 ns. The interface charge densities are considered to be 50%. The LED chip size is $300 \mu\text{m}^2$.

Results and Discussions

Band Energy Diagram and Internal Quantum Efficiency

The energy band diagram and IQE of an AlGaN/AlN nanowire UV LED are essential characteristics for providing an insight into inherent nanowire properties.

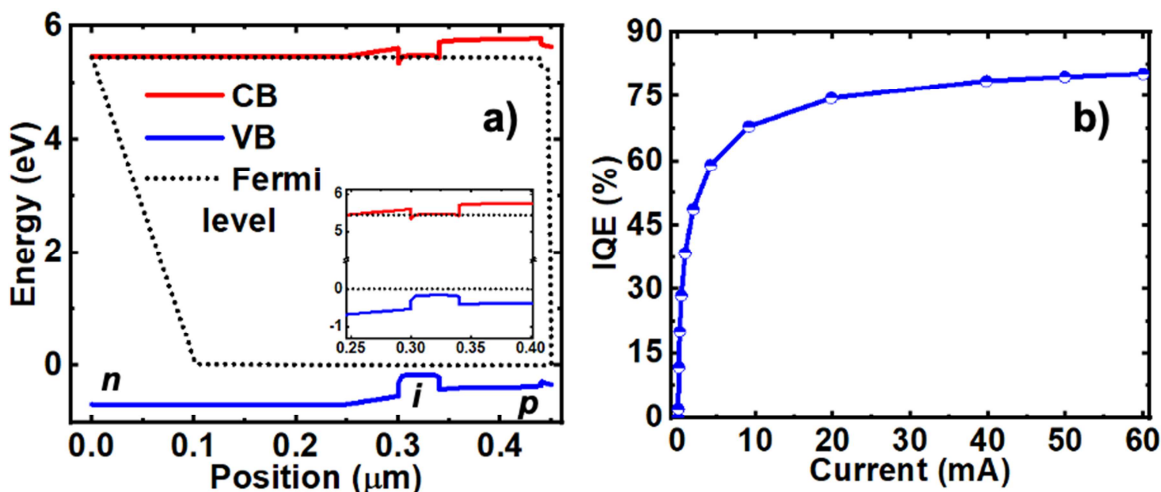


Figure 2. Energy band diagram (a) and IQE (b) of the AlGaN nanowire far-UVC LED.

Figure 2(a) shows the calculated band-energy diagram of the *n-i-p* AlGaN/AlN nanowire far-UVC LED at a 60 mA injection current. The inset shows that at the *n*-AlN/*i*-AlGaN interface, closely toward the *n*-side, the conduction band is bended down while the valence band is curved up. Due to the single quantum well and nanowire structure, the strain induced piezoelectric polarization is small, and only the spontaneous polarization mainly affects the performance of the device. In order words, the hole and electron carriers are accumulated in the same side of the quantum well, so their wave functions are

likely overlapped, leading to a high radiative recombination rate. Therefore, the radiative recombination proportion is as high as ~80% at 60 mA injection current, as shown in Figure 2(b). The IQE increases from 65% at 10 mA to reach a maximum value of 80% at 60 mA without efficiency droop.

I-V Characteristic and Output Power

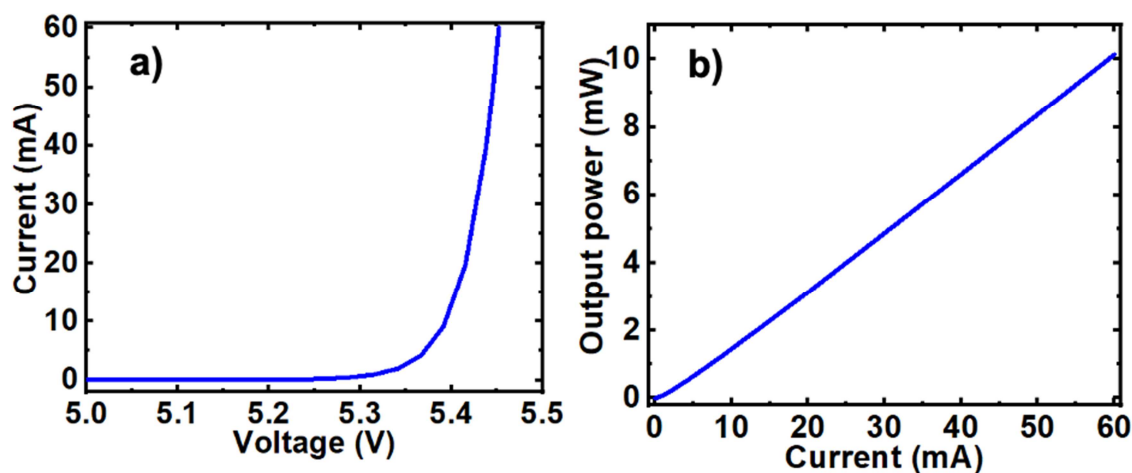


Figure 4. The I-V characteristic (a) and output power (b) of AlGaIn/AlN nanowire far UVC LED.

The current-voltage (I-V) characteristic and the output power are quantitatively determined and presented in Figure 4. Figure 4(a) shows an exponential increase in the injection currents as a function of the forward voltage. There is almost no change in the current value when the applied voltage is smaller than 5.3 V. However, a small increase by ~0.1 V in the operation voltage to 5.45 V leads to an exponential rise in the injection current, from below 5 mA to more than 60 mA, indicating a relatively small resistivity value of [17]. For example, the bias voltage at 5.35 V (V_T), defined as the threshold voltage, produces a current of 5 mA and at 5.45 V the current of 60 mA are recorded, respectively. Figure 4(b) shows a linear dependence of the output power on the injection current. The output power increases from 1.75 mW to 10 mW with increasing current from 10 mA to 60 mA.

Optical Bandpass Filter

An optical band pass filter is a structure that eliminates most wavelengths, except a narrow interval with a very high transmission. The narrow spectral LED is ideal for airborne and surface disinfection applications since the precise stimulation could be achieved when targeted molecules or events merely interact with photons at particular energy levels. The LEDs integrated with a bandpass filters would create the narrow-band LEDs. The bandpass filter is usually developed from a number of Metal/Dielectric/Metal layers. It is based on the typical metal-dielectric Fabry-Perot interferometer structures. Shown in Figure 5(a) is the design of a bandpass interference filter consisting of three Al/MgF₂/Al periods after the optimization by calculation by OpenFilters software [18]. Al and MgF₂ are common materials for making band pass filters in UV wavelengths. MgF₂ which is transparent in a wide range from 210 nm to 10 μ m [19] is used as the spacer, and aluminum plays a role as mirrors. Al metal is superior reflective in the far-

UVC wavelength, compared to other common reflective metals [20]. The designed bandpass filter includes three MgF_2 layers sandwiched by four parallel Al layers. The thickness of the filter is ~ 265 nm, shown in Figure 5(a). This bandpass filter is easily fabricated and it results in a relatively high transmission of up to 50% at 222 nm with a FWHM of ~ 12 nm, presented in Figure 5(b). The numerically realized bandpass filter shows promising for narrow far-UVC LEDs. The far-UVC LEDs pave the way for effectively disinfecting airborne and surface pathogen organisms without harmful effect and phototoxicity in occupied spaces. For example, 222 nm UV LEDs with its FWHM of 12 nm. Its spectrum is from 209.5 nm to 234.5 nm. Photon energy in the far-UVC wavelengths, highly absorbed by the layer of dead skin cells, will be safer than the longer wavelength LEDs. For example, 254 nm UV LED is able to penetrate deep into the dermis, causing detrimental health problems [21].

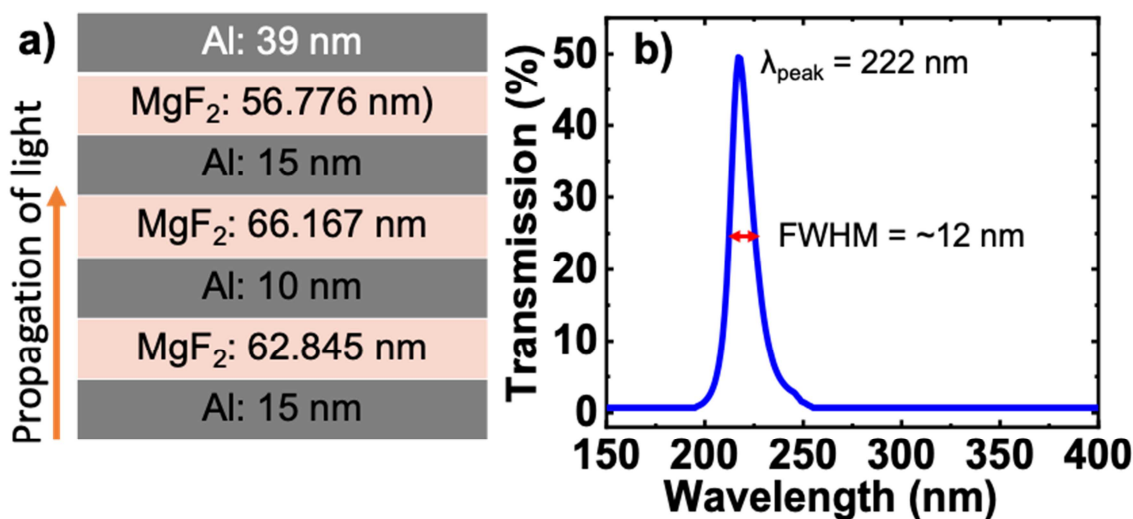


Figure 5. The bandpass filter of three periods of Al/ MgF_2 /Al layers (a), and (b) the obtained narrow spectrum from the filter at 222 nm.

Conclusion

In this study, we have designed a simple *n-i-p* AlGaIn nanowire far-UVC LED, with a single quantum well for the emission at 222 nm. The IQE of 80% and the corresponding output power of 10 mW with an excellent I-V characteristic suggest a remarkable design for AlGaIn/AlN nanowire far-UVC LEDs. Such far-UVC LED chips are also able to be integrated with a bandpass UV filter for a narrow-spectral emission. The FWHM of the obtained narrow-far-UVC LED is as small as ~ 12 nm, superior to the current broadband far-UVC LEDs for the airborne and surface disinfection.

Acknowledgements

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