Supplementary Information

Aluminum nitride nanowire light emitting diodes: Breaking the fundamental bottleneck of deep ultraviolet light sources

S. Zhao,[1] A. T. Connie,[1] M. H. T. Dastjerdi,[1] X. H. Kong,[2] Q. Wang,[1] M. Djavid[1], S. Sadaf,[1] X. D. Liu,[3] I. Shih,[1] H. Guo,[2] and Z. Mi[1]*

[1] *Department of Electrical and Computer Engineering, McGill University, 3480 University Street, Montreal, Quebec, Canada H3A 0E9*

[2] *Department of Physics, McGill University, 3600 University Street, Montreal, Quebec, Canada H3A 2T8*

[3] *Facility for Electron Microscopy Research, McGill University, 3640 University Street, Montreal, Quebec H3A 0C7*

*E-mail: zetian.mi@mcgill.ca

1. Ab-initio calculation on Mg doping into AlN nanowires

To further understand the mechanism of Mg dopant incorporation in AlN nanowires, we have performed the first-principle calculation on *m*-planes (nanowire sidewalls) using the Vienna Ab-initio Simulation Package (VASP). The calculations were performed on a 4×4 superlattice with the asymmetric slab mode. The vacuum layer thickness is 20 Å. Surface reconstruction was considered in the calculation and functional hydrogen was employed to saturate dangling bonds. The structure used for the calculation is shown in Fig. S1a, and doping position index n = 1 indicates the surface. The Mg formation energy for each layer is shown in Fig. S1b, and it is seen that the near-surface region (n = 3) has much lower formation energy compared to that in the bulk region (e.g., n = 7). This will lead to Mg surface preferential incorporation. However, as discussed in the main text, to realize p-type doping, the Mg surface incorporation rate has to be larger than the Mg surface desorption rate.

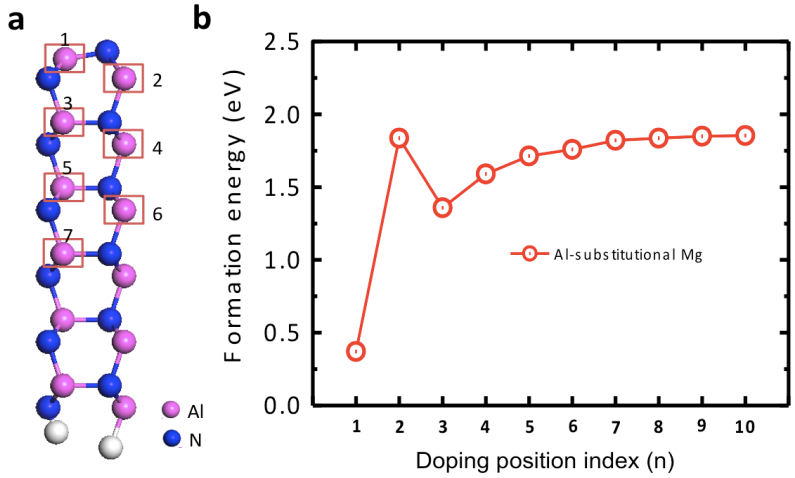

Figure S1 | ab-initio calculation of Mg doping into AlN nanowires. (**a**) Illustration of the structure used for calculation. (**b**) Al-substitutional Mg formation energy along the nanowire radial direction. The doping position index n = 1 indicates the surface. It is seen that the near-surface region has much lower formation energy than in the bulk region.

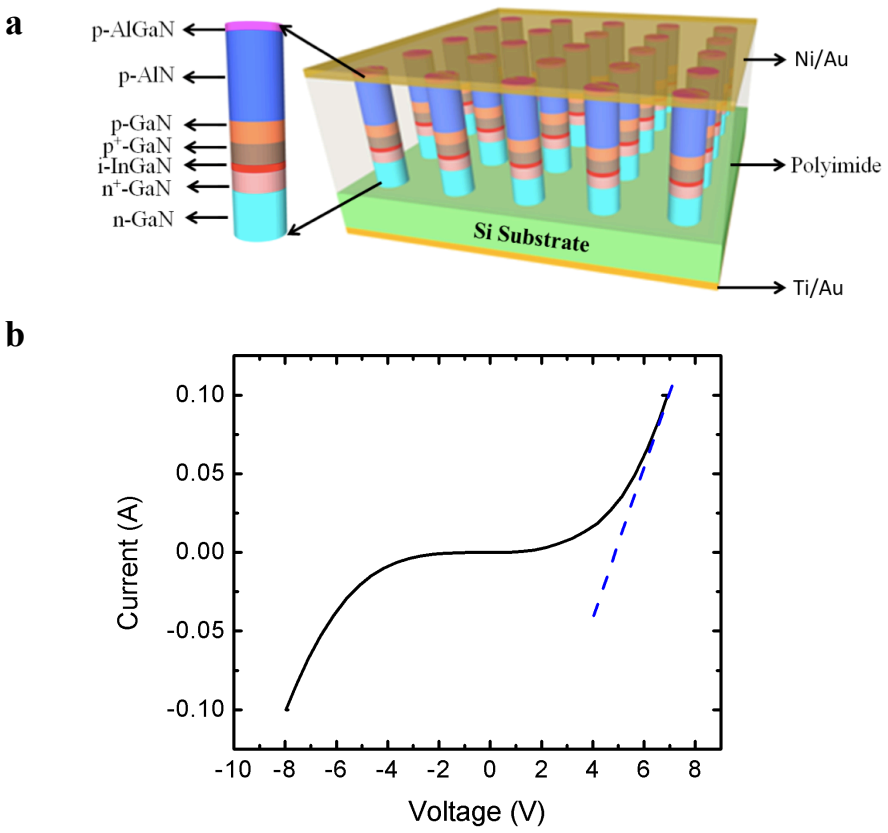

Figure S2 | The structure used to estimate the hole concentration in AlN:Mg nanowires. (**a**) A schematic of the device structure used to estimate free hole concentration in AlN:Mg nanowires. (**b**) Room temperature *I-V* characteristics of the device.

2. Free hole concentration estimation

The free hole concentration in AlN LEDs was estimated by the nanowire structure as described in Fig. S2a, which consists of heavily doped n-type Si substrate, a n^+-GaN/InGaN/p^+-GaN tunnel junction, a 30 nm p-GaN buffer layer to minimize any effect p-AlN on GaN/InGaN tunnel junction, a 45 nm Mg-doped AlN section with similar growth parameters as used in growing the p-type section in AlN LEDs, and a 10 nm p-type AlGaN contact layer similar to the growth conditions used in the AlN LEDs. The room temperature *I-V* characteristics are shown in Fig.

S2b. For a device with a size of 0.3 mm by 0.3 mm, the resistance estimated by the slope (dash line in Fig. S2b) in the forward bias condition is 27 Ω.

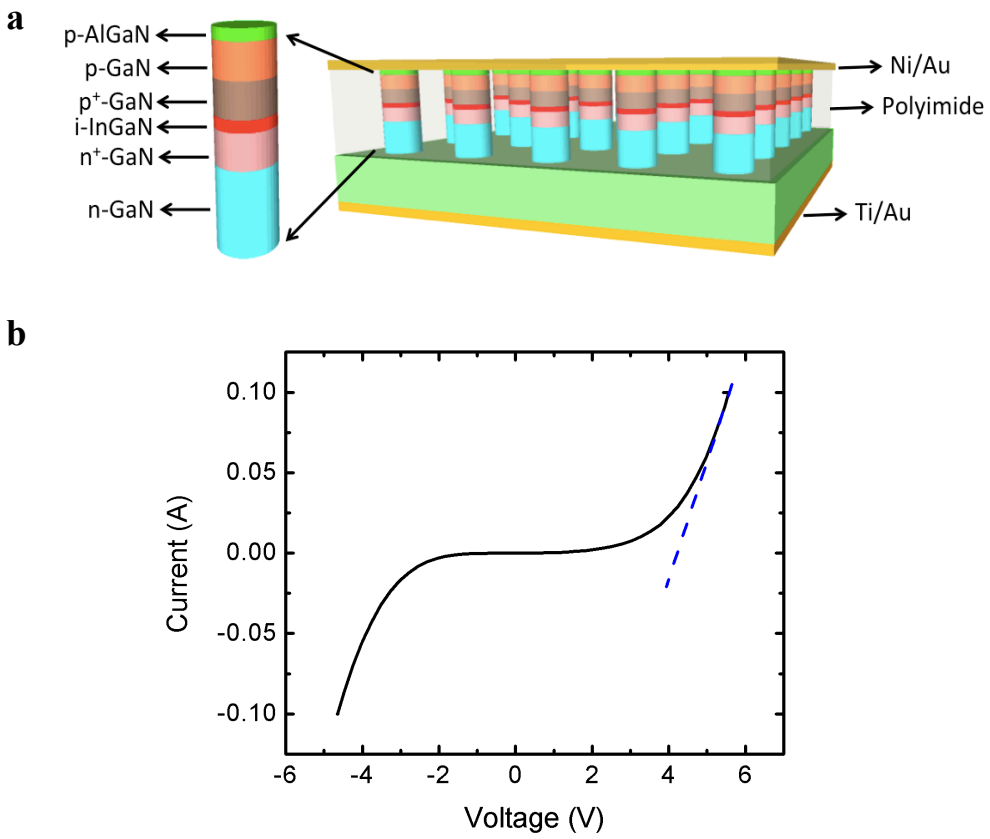

Figure S3 | Estimation of the background resistance (without AlN:Mg section) for the device structure shown in Fig. S2a. (**a**) A schematic of the device structure. (**b**) Room temperature *I-V* characteristics.

In order to provide a more accurate estimation of the resistance of the AlN:Mg section in the structure shown in Fig. S2a, another identical structure but without the AlN:Mg section is fabricated, illustrated in Fig. S3a. Such a device provides the background resistance. The *I-V* characteristics are shown in Fig. S3b, and the resistance of this calibration structure is estimated to be 19 Ω by the linear part marked by the dash line.

From the resistance difference calculated from Fig. S2b and S3b, the resistance of AlN:Mg section can be derived to be 8 Ω. With a device size of 0.3 mm by 0.3 mm, a fill factor of 0.3 estimated from the top view SEM image, and assuming a hole mobility of 1 cm^2/V cm in the high end[1], the room temperature free hole concentration is estimated to be 1×10^{16} cm^{-3}, or higher, for AlN:Mg nanowires.

3. Supporting Figures

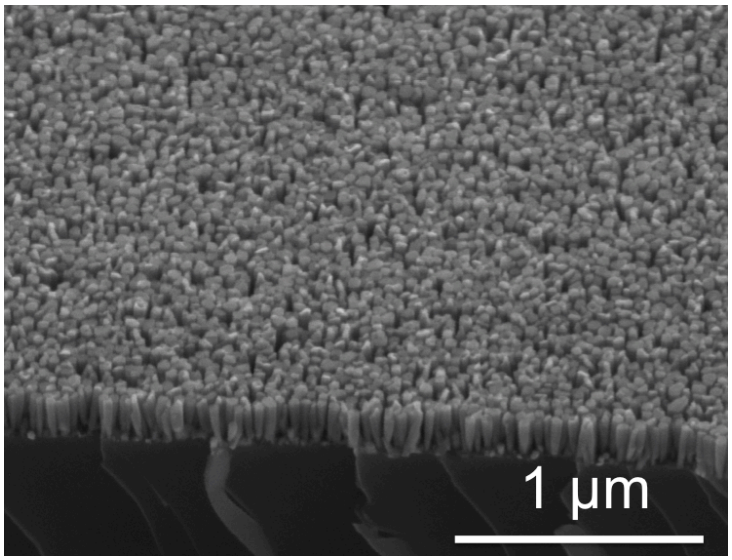

Figure S4 | An SEM image of AlN LEDs on Si taken with a 45-degree angle (juxtaposed against Fig. 3a in the main manuscript).

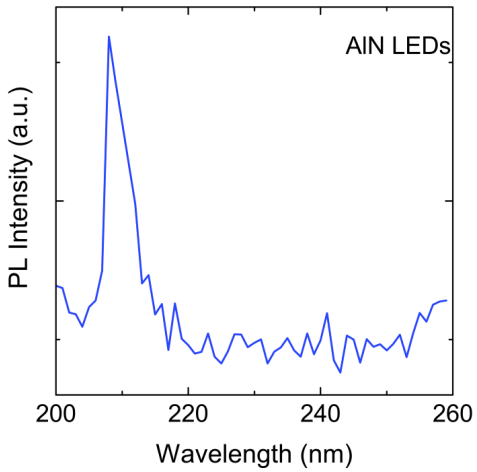

Figure S5 | A photoluminescence spectrum of AlN LEDs taken at room temperature with an excitation power of 1 mW.

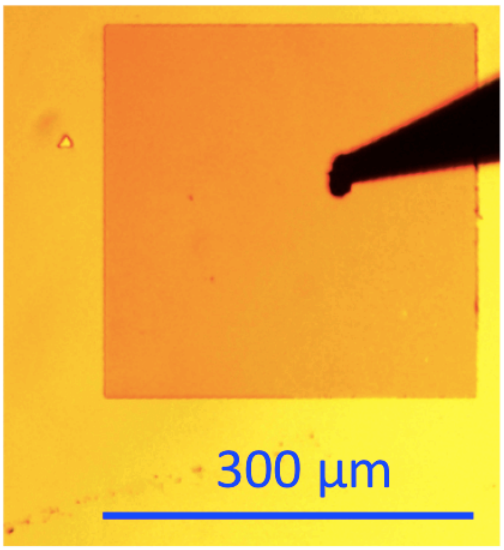

Figure S6 | A top view optical image of fabricated AlN LEDs (size 0.3 mm by 0.3 mm).

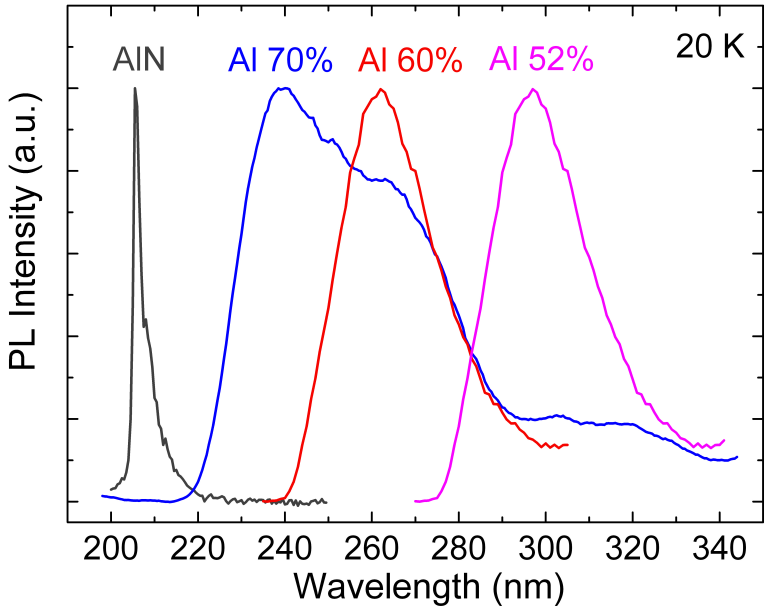

Figure S7 | Photoluminescence spectra measured at 20 K with an excitation of 1 mW for Al(Ga)N LED structures with different Al concentrations. It is seen that by changing the Al concentration, the emission wavelength can be tuned from 210 nm to 300 nm.

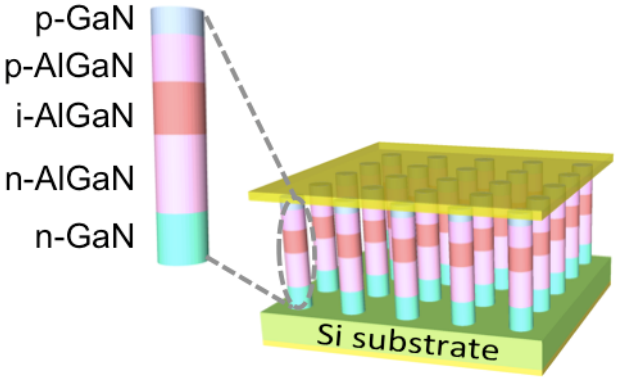

Figure S8 | A schematic plot of the AlGaN DUV LEDs (juxtaposed against Fig. 3d in the main manuscript). From bottom to top it consists of heavily doped Si substrate, Si-doped GaN, n-AlGaN, AlGaN active region, p-AlGaN, and Mg-doped GaN as the contact layer.

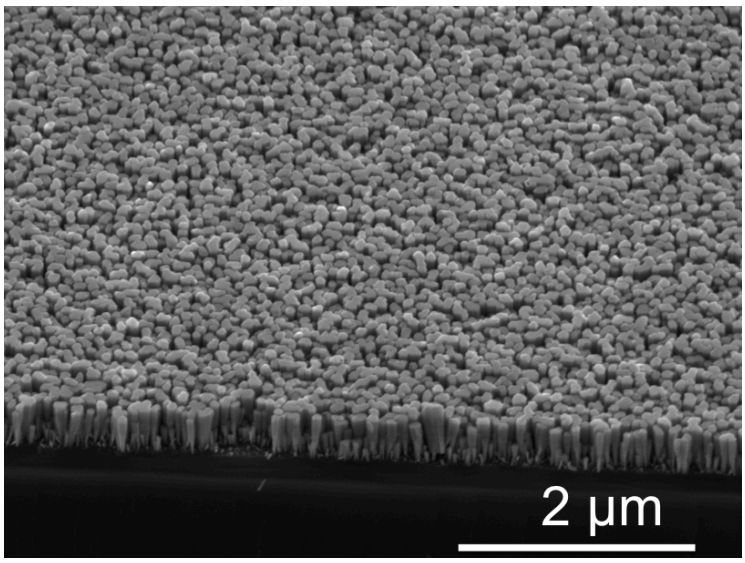

Figure S9 | An SEM image of AlGaN LEDs on Si taken with a 45-degree angle (juxtaposed against Fig. 3d in the main manuscript).

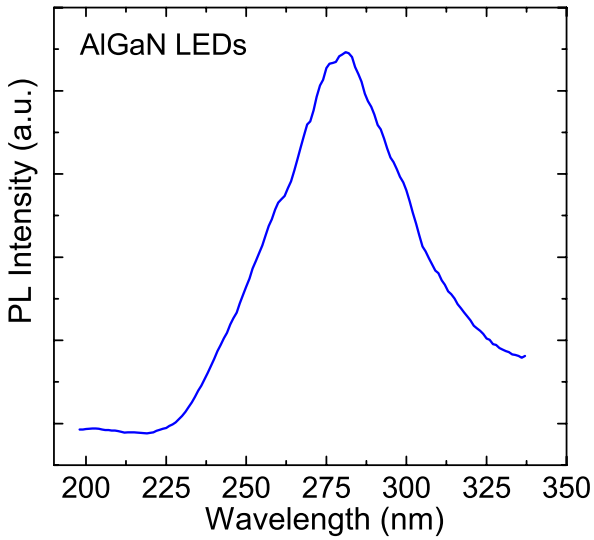

Figure S10 | A photoluminescence spectrum of AlGaN LEDs taken at room temperature with an excitation power of 1 mW. The nominal Al concentration is estimated to be 72 % by Al/(Al+Ga) flux ratio.

References

1 Taniyasu, Y., Kasu, M. & Makimoto, T. An aluminium nitride light-emitting diode with a wavelength of 210 nanometres. *Nature* **441**, 325-328 (2006).