

ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Lateral-Polarity Structure of AlGa_N Quantum Wells:
A Promising Approach to Enhancing the Ultraviolet
Luminescence

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Title Lateral-Polarity-Structure of AlGa_N Quantum Wells: A Promising Approach for Enhancing the Ultraviolet Luminescence

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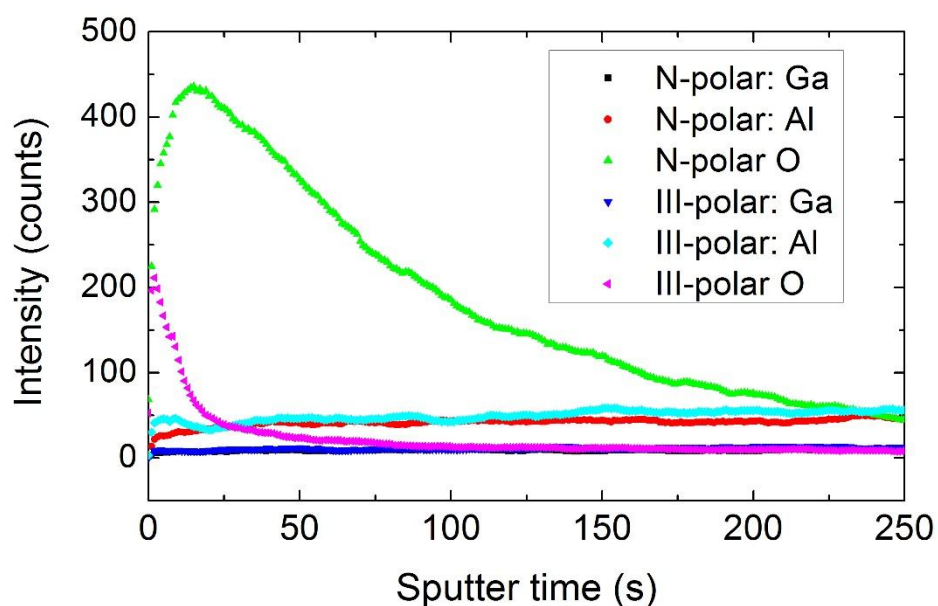


Figure S1. SIMS analysis of Ga, Al and O concentrations inside N-polar and III-polar domains of LPS sample. Y axis represents the counts of collected SIMS signal, which is proportional to atom concentration. The polarity has significant influence on the incorporation of native and extrinsic defects. More than 10 times higher oxygen concentration in N-polar domains was observed from SIMS measurement and it was widely expected in the N-polar nitride films, as reported by others experimentally [¹⁻⁴] and explained by density-functional theory.[⁵⁻⁶]

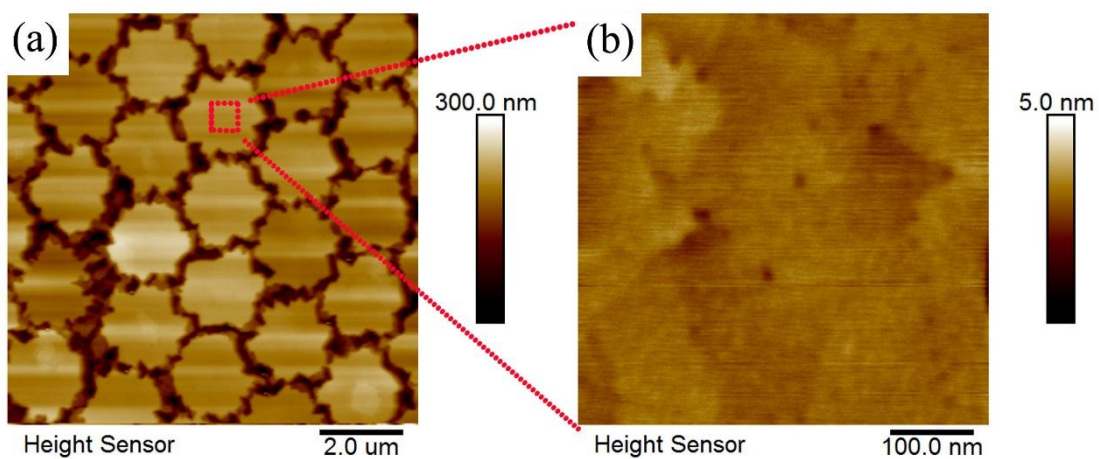


Figure S2. AFM image of as-grown LPS with 2 μm periodicity (a). Zoom-in view of the III-polar region as indicated in the red circle in a, revealing atomically smooth surface with RMS roughness of only 0.72 nm (b)

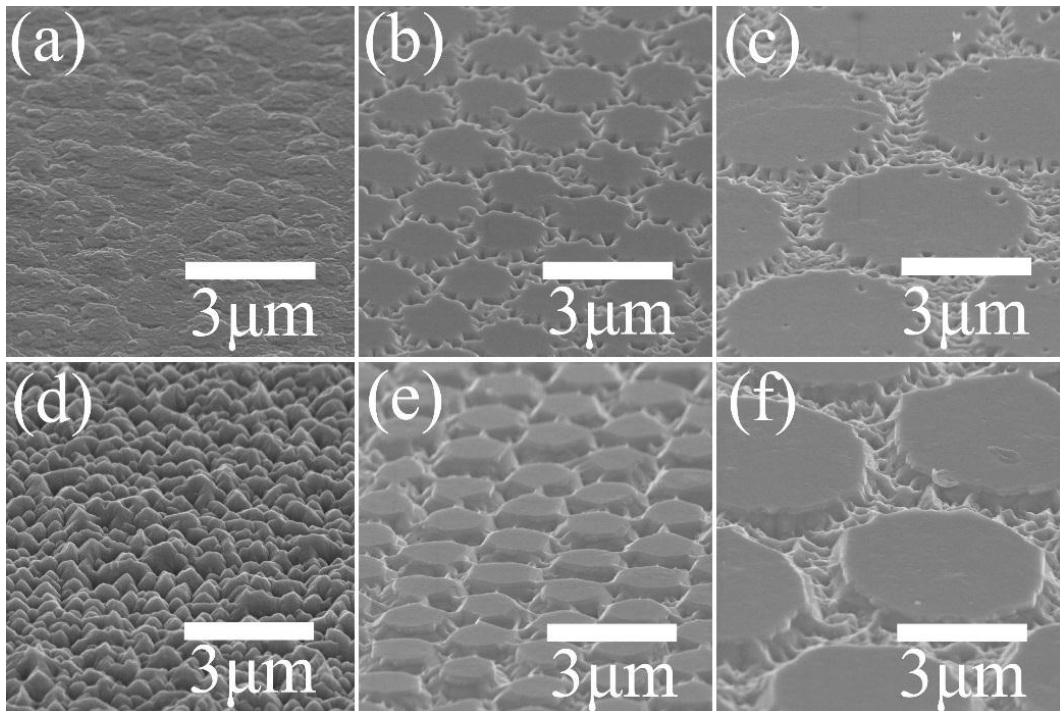


Figure S3. 30° tilted view SEM images of as-grown LPS AlGaIn MQWs (a-c) and after 3mol/L KOH etching for 5min (e-f) with periodicities of 300 nm (a,d), 2 μm (b,e) and 6 μm (e,f), respectively. After KOH etching, LPS grown on the patterned AlN buffer with 2 μm and 6 μm periodicities exhibit nanopillar structures as a result of etching selectivity between N-polar and III-polar domains. However, in the case of LPS with 300 nm periodicity, since the patterned LT-AlN buffer layer is quite thin (~15 nm, data not shown) to begin with due to RIE over-etching, AlGaIn MQW grown on top of it exhibits a rough surface (Figure S1(a)), which is characteristic of a uniform N-polar film. After KOH etching, the surface is covered with random distributed etching hillocks.

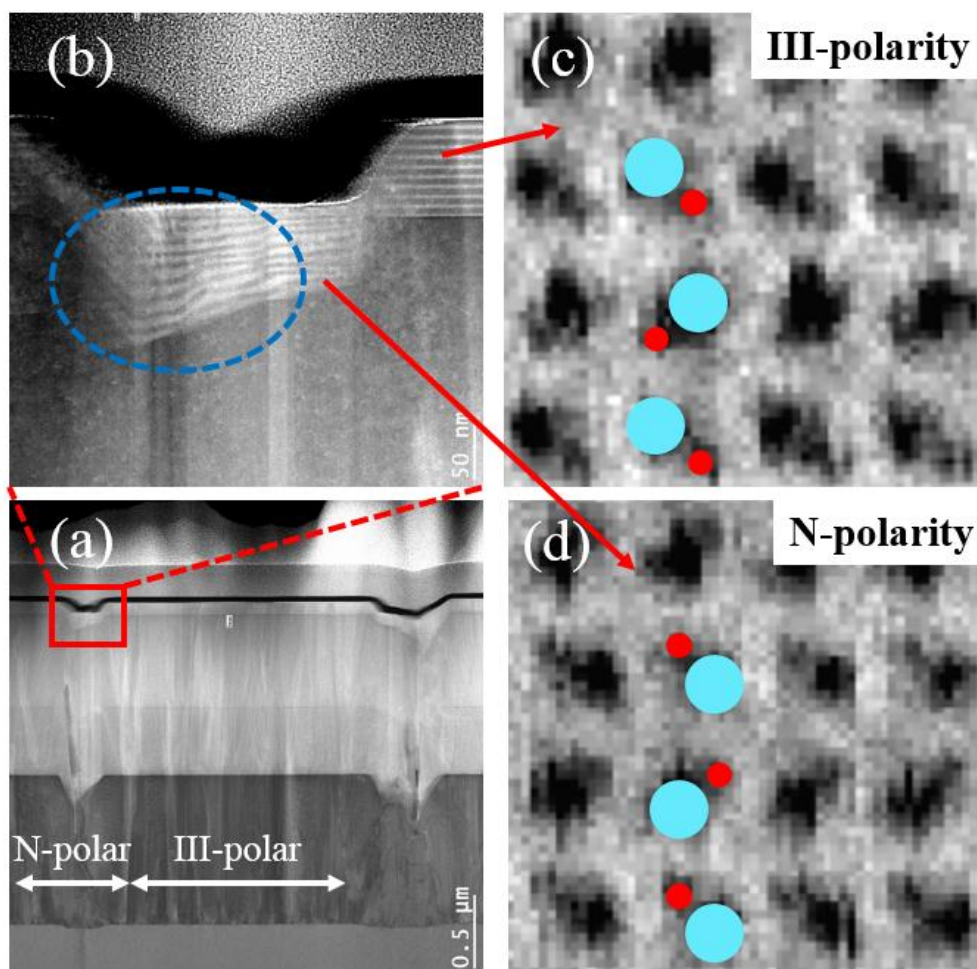


Figure S4. STEM image at another location of the LPS MQWs. Low magnification image of the sample with 2 μm periodicity (a); Zoom-in view of the N-polar MQWs from the red square marked in a (b); Atomic resolution STEM images in the III-polar (c) and N-polar (d) domains. Blue and red dots represent metal atoms and nitrogen atoms, respectively. Note that QBs and QWs have zig-zag shapes in the region in dashed blue circles from (b), even though the surface is flat. This indicates a 3D growth mode in N-polar domains and local compositional inhomogeneities of the MQWs, which leading to enhanced photoluminescence.

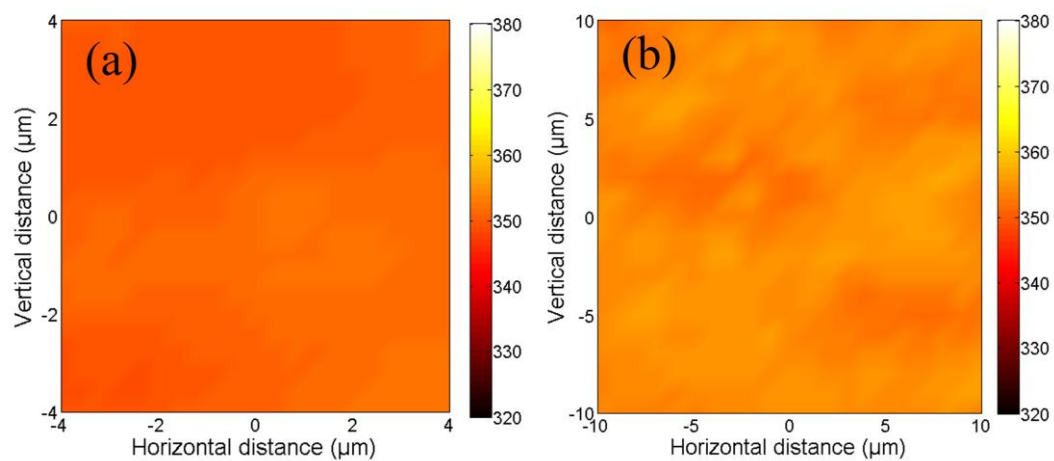


Figure S5 Space-resolved PL position mapping of LPS with 2 μm (a) and (b) 6 μm periodicity. Color bar represents the peak position ranging from 320 to 380 nm. Peak positions remain nearly identical for LPS with 2 and 6 μm periodicity, and no obvious trend was observed

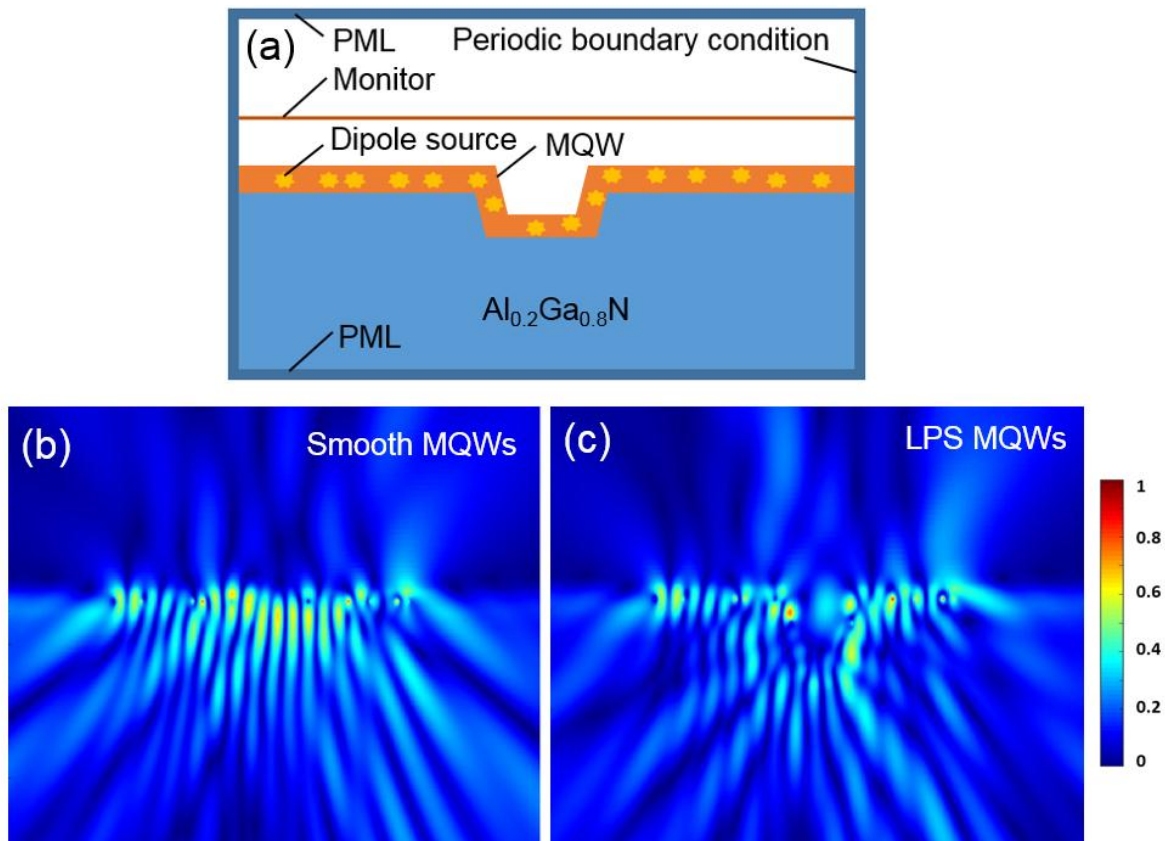


Figure S6 The schematic of the simulation setup for the LPS MQW with inverted truncated pyramid in the center (a). Comparison of electric field intensity and distribution in the smooth MQWs (b) and LPS MQWs with trench like N-polar domains (c). The refractive index of $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$, $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$, and GaN are taken as 2.40, 2.50 and 2.64 respectively⁷. Periodic boundary conditions are applied on the left and right hand side of the simulation area to account for the large size of the actual device. Perfectly matched layer (PML) boundary conditions are applied at the top and bottom of the simulation area to absorb the escaping light. A total number of 10 incoherent broadband dipole source is placed randomly inside $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}/\text{GaN}$ MQWs. The monitor placed at the top of the MQWs is used to collect the light extracted from the MQWs. The thickness of each layer and dimensions were chosen to match the TEM measured data (depth is ~ 250 nm and width is ~ 300 nm).

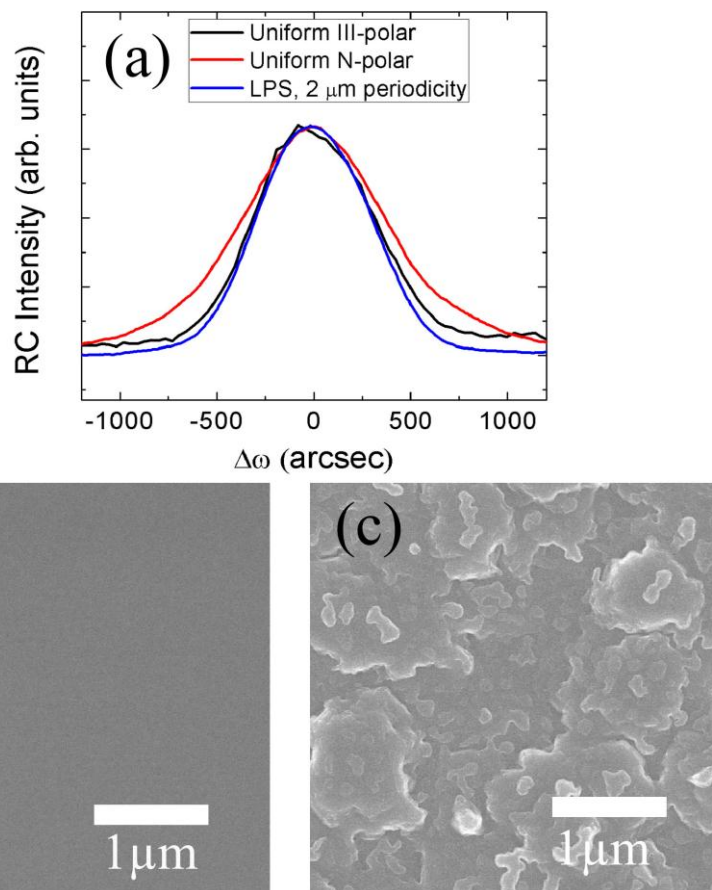


Figure S7. Symmetric (002) XRD rocking curve scans of the MQWs from uniform III-polar, N-polar and LPS with 2 μm periodicity, FWHM values are 601, 783 and 571 arcsec, for uniform III-polar, N-polar and LPS MQWs, respectively(c); SEM images of uniform III-polar (b) and N-polar (c) MQWs. A particle shown in (b) suggests the smoothness of uniform III-polar surface

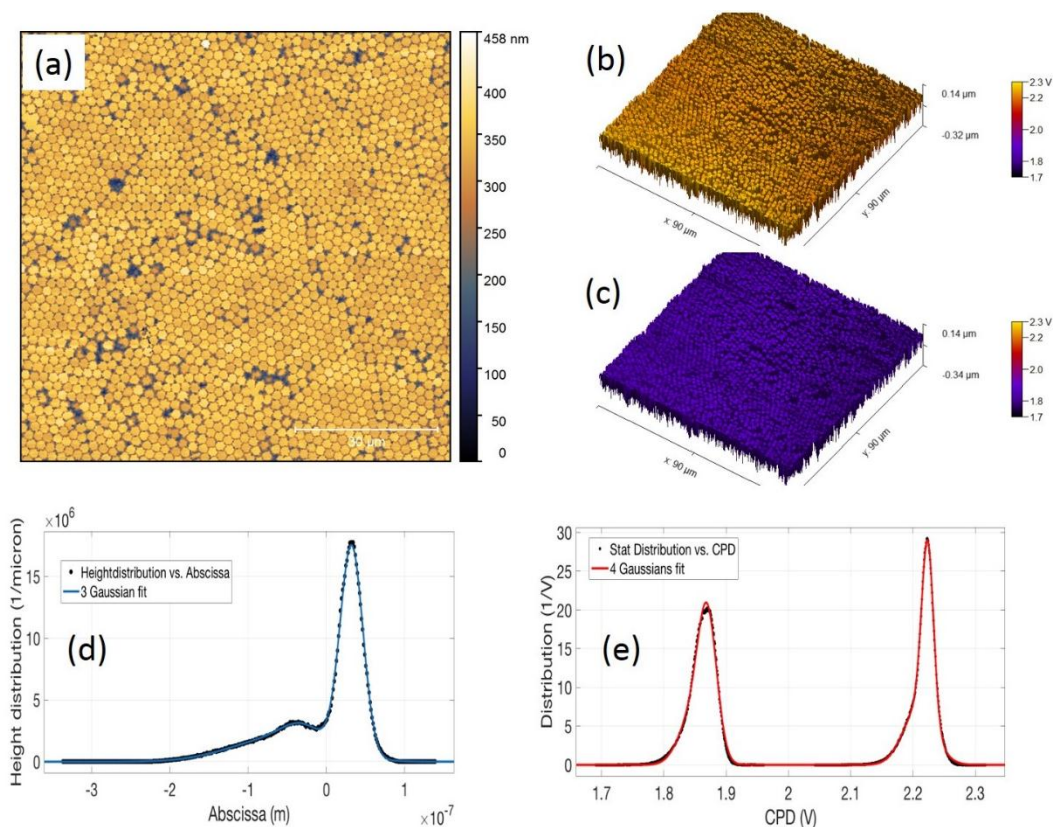


Figure S8 (a) Topography of $90 \times 90 \mu\text{m}^2$ region in which SKPM study under UV illumination (b) and dark (c) have been performed. (d) Statistical distribution of height values (black dots) with the 3 Gaussian best fits (blue line) superimposed. (e) CPD distributions (black dots) for Dark (left one, CPD <2V) and UV (right one, CPD >2V); the two distributions appear well separated with no overlapping. The red line shows the best 4 Gaussian peaks fitting, where 2 Gaussians well describe each distribution. To determinate the SKPM values distribution under UV illumination ($4.9 \mu\text{W}/\text{cm}^2$, corresponding to the 80% of the maximum CPD photoresponse detected) and dark conditions, we acquired surface potential signal on the same $90 \times 90 \mu\text{m}^2$ shown in Figure S3 (a), where the III-polar and N-polar domains are clearly visible as flat top areas and valleys and whose statistical inference is shown by the height values in (d), well described by three Gaussian distributions (see Table S1). CPD values under UV and dark conditions are shown in (b), (c) as color rendering on 3D topography to directly show their spatial localization. Notice that the color scales in the two images are the same, to highlight the full range variation due to photo-generated charges. CPD distributions for dark and UV are plotted in (e). These are well represented by two Gaussian distributions each.

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