

Supporting information

Single p-n Homojunction White Light Emitting Diodes Based on High-performance Yellow Luminescence of Large-Scale GaN Microcubes

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The X-ray rocking curves of GaN samples grown on Si substrates

Rocking curves were recorded using a Bruker-AXS D8-Discover diffractometer equipped with parallel incident beam, a vertical θ - θ goniometer, a XYZ motorized stage and a General Area Diffraction Detection System. The X-ray diffractometer was operated at 40 kV and 40 mA to generate Cu $K\alpha$ radiation.

As we all know, since lattice-matched substrates are not readily available, heteroepitaxial growth of GaN on lattice-mismatched substrates such as GaAs and Al_2O_3 has been a common method, resulting in misfit strain. This misfit strain induces structural imperfections such as threading dislocations, stacking faults, etc, depending upon the particular strain relief mechanism^{1, 2}. The high dislocation density is not conducive to the fabrication of high-performance GaN based devices with long lifetime³. To further identify the crystalline quality, the structural properties of the GaN samples were analyzed by a high-resolution X-ray diffraction (HRXRD) rocking curve. Figure S1a depicts the ω -scan spectra of the (222) planes of c-GaN crystals grown on Si (111) substrates and the FWHM of the (222) peak is 162 arcsec for c-GaN grown on Si (111). Figure S1b,c represent the X-ray rocking curves for the symmetric (004) plane and the asymmetric (102) plane of h-GaN grown on Si (101), from which the values of FWHM for the symmetric (004) plane and the asymmetric (102) plane are 228.2 and 249.3 arcsec, respectively. It is well known that the FWHM of the (102) reflection corresponds to the lattice distortion from all components of the threading dislocations including pure edge, screw and mixed screw-edge dislocations, while the FWHM of (004) reflection is

associated with screw and mixed screw-edge dislocations⁴. These values of FWHMs are comparable to the state-of-art values of GaN-based LED wafers on graphene or hexagonal boron nitride nanosheets substrate grown by hydride vapor phase epitaxy methods², suggesting high crystallinity GaN samples have been grown on Si substrates using a simple chemical vapor deposition method. The lower FWHM values of the (222) peak of the c-GaN, (004) and (102) peaks of the h-GaN crystals grown on Si substrates also suggest that there are fewer threading dislocations. The densities of dislocations in GaN can be approximately evaluated as functions of FWHM from the following equation^{4, 5}

$$D = \frac{\beta^2}{9b^2}$$

where D is the dislocation density, β is the FWHM value of HRXRD peaks, and b is the length of the Burger vector of the corresponding dislocation. We can therefore calculate the dislocation density of GaNs grown on the Si (111) and Si (101) substrates are $1.10 \times 10^7 \text{ cm}^{-2}$, $8.5 \times 10^7 \text{ cm}^{-2}$ and $8.9 \times 10^7 \text{ cm}^{-2}$, respectively. This once again confirms the high crystalline quality of as-grown GaN samples.

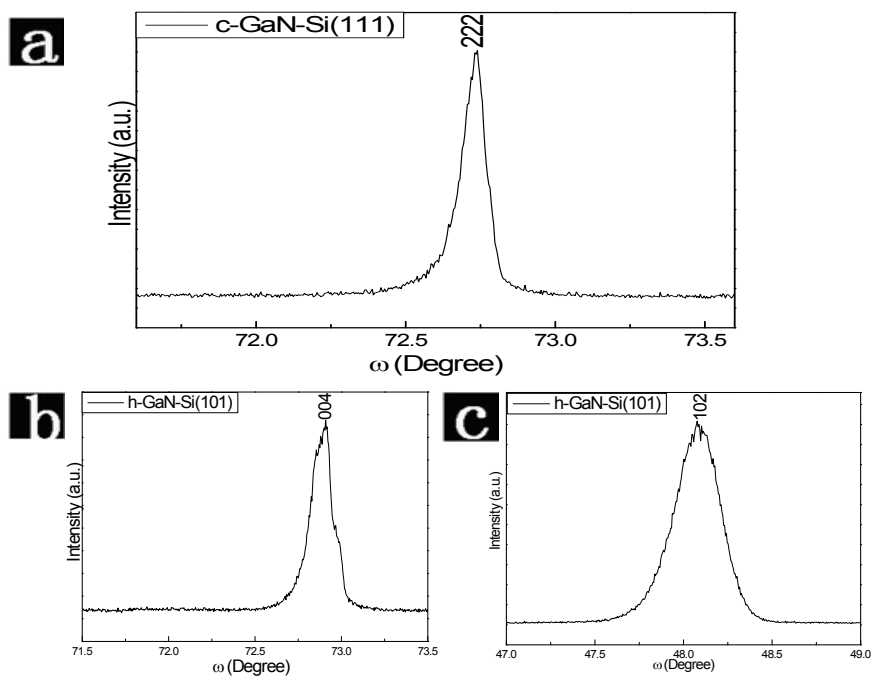


Figure S1 X-ray rocking curves for (a) the (222) plane of c-GaN grown on Si (111) substrates (b) the symmetric (004) plane of h-GaN grown on Si (101) substrates (c) the asymmetric (102) plane of h-GaN grown on Si (101) substrates

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