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Citation:

Chen, Pei-Yu, Agham B. Posadas, Sunah Kwon, Qingxiao Wang, et al. 2017. "Cubic crystalline erbium oxide growth on GaN(0001) by atomic layer deposition." Journal of Applied Physics 122(21), doi:10.1063/1.4999342

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Supplementary Material

Cubic Crystalline Erbium Oxide Growth on GaN(0001) by Atomic Layer Deposition

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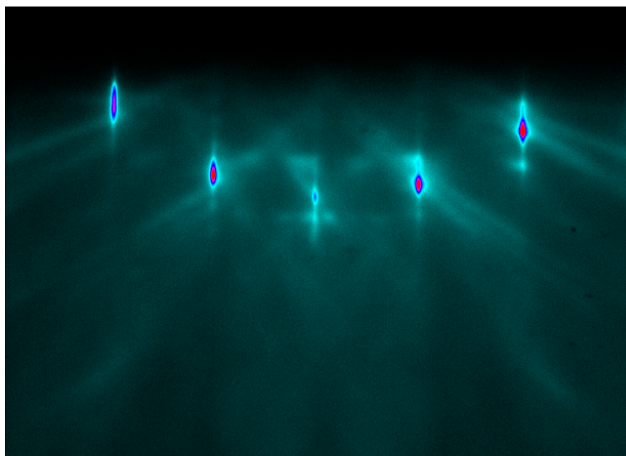

FIG. S1. RHEED image of GaN substrate cleaned by chemicals (acetone, isopropyl alcohol, deionized water, HCl, and NH_4OH in sequence) and N_2 plasma. The image shows a 1×1 surface along the <11-20> azimuth.

Supplementary Calculation I:

Theoretical lattice mismatch between a cubic structure and a wurtzite structure can be calculated by finding the matching surface unit cells at a superlattice distance.[1] For the C-Er_2O_3/GaN heterostructure, the GaN(0001) and C-Er_2O_3(111) planes are aligned from XRD measurements (Fig. 3) and this alignment leads to $\sqrt{2} \times a_{Er2O3}$ (a_{Er2O3} = 10.547 Å) as the in-plane $a_{IP\text{-}Er2O3}$. A superlattice with five times the GaN lattice constant (a_{GaN} = 3.189 Å) is found to match $a_{IP\text{-}Er2O3}$ the best. Using five times the GaN lattice constant leads to a lattice mismatch of +6.90% as shown below.

$$Mismatch = \frac{3.189 \times 5 - \sqrt{2} \times 10.547}{\sqrt{2} \times 10.547} \times 100\% = 6.90\%$$

The corresponding crystal structure viewed along C-Er_2O_3<111> || GaN<0001> is also simulated by VESTA[2] to examine the lattice mismatch between C-Er_2O_3 and GaN, as shown in Fig. 8. The lattice mismatch along GaN<11-20> and GaN<1-100> directions are estimated as follows.

<u>Along GaN<11-20></u>:

d_{Ga-Ga} = 3.189 Å

$d_{Er_2O_3(-220)}$ = 3.729 Å

From Fig. 8, coincidence of Er atoms with Ga atoms along the GaN<11-20> direction leads to $5 \times \overline{Ga - Ga} \cong 4 \times \overline{Er - Er}$. Therefore, five times of d_{Ga-Ga} is used to compare with four times of $d_{Er_2O_3(-220)}$, which results in the lattice mismatch of +6.90%.

$$Mismatch = \frac{3.189 \times 5 - 3.729 \times 4}{3.729 \times 4} \times 100\% = 6.90\%$$

<u>Along GaN<1-100></u>:

d_{Ga-Ga} = 5.524 Å

$d_{Er_2O_3(-422)}$ = 2.153 Å

From Fig. 8, coincidence of Er atoms with Ga atoms along the GaN<1-100> direction leads to $3 \times \overline{Ga - Ga} \cong 7 \times \overline{Er - Er}$. Similarly, the lattice mismatch of +9.96% is obtained by using three times of d_{Ga-Ga} and seven times of $d_{Er_2O_3(-220)}$.

$$Mismatch = \frac{5.524 \times 3 - 2.153 \times 7}{2.153 \times 7} \times 100\% = 9.96\%$$

Supplementary Calculation II:

The lattice mismatch at various temperatures can be estimated by utilizing the coefficient of thermal expansion, α. The thermal expansion coefficients for Er_2O_3 and GaN are 7.25×10^{-6} K^{-1} and 5.59×10^{-6} K^{-1}, respectively.[3-4] With $\left(\frac{\Delta L}{L}\right) = \alpha \Delta T$ and five times the multiple of the GaN, lattice constants and lattice mismatch can be calculated at the 250 ˚C ALD growth temperature and the 600 ˚C post-deposition annealing temperature.

<u>At room temperature of 25 ˚C</u>:

$$Mismatch = \frac{3.189 \times 5 - \sqrt{2} \times 10.547}{\sqrt{2} \times 10.547} \times 100\% = 6.90\%$$

<u>At the deposition temperature of 250 ˚C</u>:

$$L_{GaN} = 5.59 \times 10^{-6} \times (250 - 25) \times 3.189 + 3.189 = 3.193$$

$$L_{Er_2O_3} = 7.25 \times 10^{-6} \times (250 - 25) \times 10.547 + 10.547 = 10.564$$

$$Mismatch = \frac{3.193 \times 5 - \sqrt{2} \times 10.564}{\sqrt{2} \times 10.564} \times 100\% = 6.86\%$$

<u>At the post-deposition annealing temperature of 600 ˚C</u>:

$$L_{GaN} = 5.59 \times 10^{-6} \times (600 - 25) \times 3.189 + 3.189 = 3.199$$

$$L_{Er_2O_3} = 7.25 \times 10^{-6} \times (600 - 25) \times 10.547 + 10.547 = 10.591$$

$$Mismatch = \frac{3.199 \times 5 - \sqrt{2} \times 10.591}{\sqrt{2} \times 10.591} \times 100\% = 6.79\%$$

The differences in lattice mismatch at various temperatures are small due to the similar coefficients of thermal expansion for Er_2O_3 and GaN. Therefore, thermal expansion is a minor contributing factor for introducing tensile strain into C-Er_2O_3 during cooling from the growth temperature and the annealing temperature to room temperature.

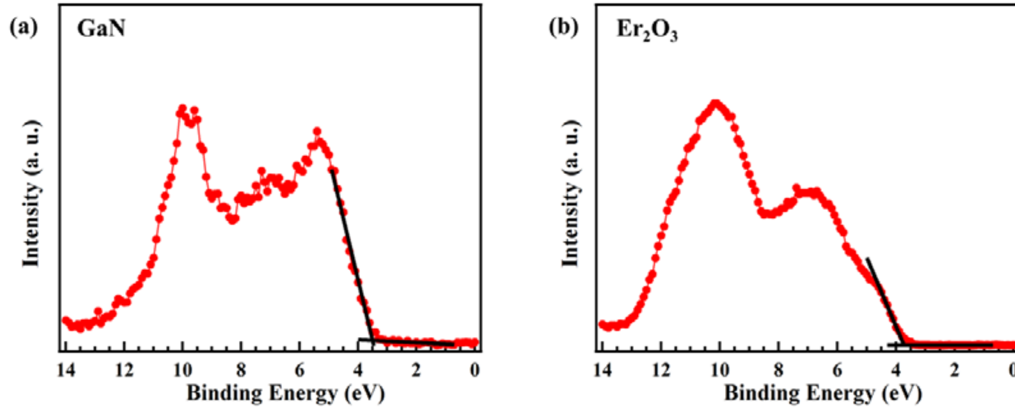

FIG. S2. The valence band spectra of (a) the clean GaN(0001) surface and (b) the 19.6-nm thick Er_2O_3 film. The VBM value is determined by extrapolating the leading edge of the valence band spectrum to the base line. The clean GaN shows a VBM binding energy of 3.50 eV, while 19.6-nm thick C-Er_2O_3 displays a VBM binding energy of 3.73 eV.

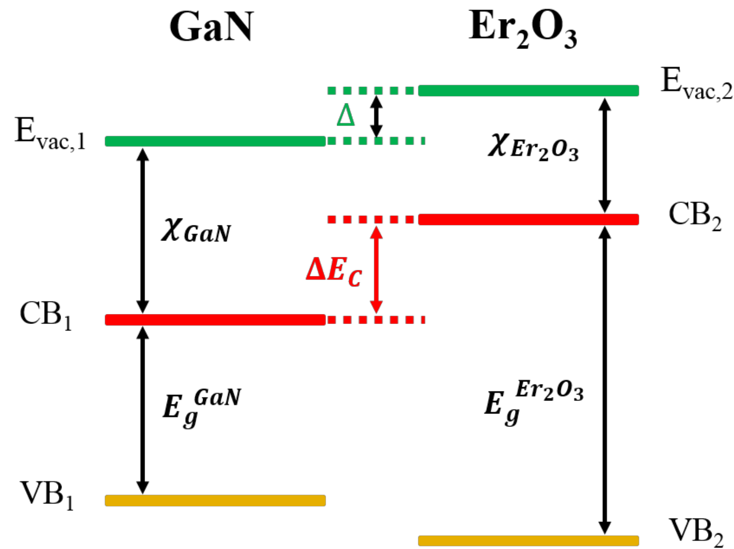

FIG. S3. The band diagram affected by the interface dipole (Δ). In this scenario the ΔE_C is increased by the presence of the positive interfacial dipole.

Supplementary Material References

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