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**Supporting Information:**

# The stacking faults annihilation in a-plane AlN during high temperature annealing

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**The 2θ-ω scan curves of a-AlN with different annealing conditions:**

The symmetric 2θ-ω scan curves of sputtered a-AlN/sapphire template with different annealing conditions are shown in Figure 1. It can be concluded that there are three strong diffraction peaks located at 25.5°, 52.6° and 59.5°, corresponding to the diffractions of (1-102)/ (2-204) r-plane sapphire substrate and nonpolar (11-20) AlN, respectively. Compared to the reflection intensity of the sputtered layer, the intensity of the peaks corresponding to (11-20) a-AlN layer is significantly increased (Fig. S1), indicating that the structural defects are smaller. In addition to the diffraction XRD peaks of sapphire and AlN, the 2θ-ω scan curve of the sample annealed at 1750 ℃ shows several peaks, which corresponding to different crystal phases of $Al_2O_3$. The results indicate that the AlN surface was oxidation and decomposition during the annealing process.

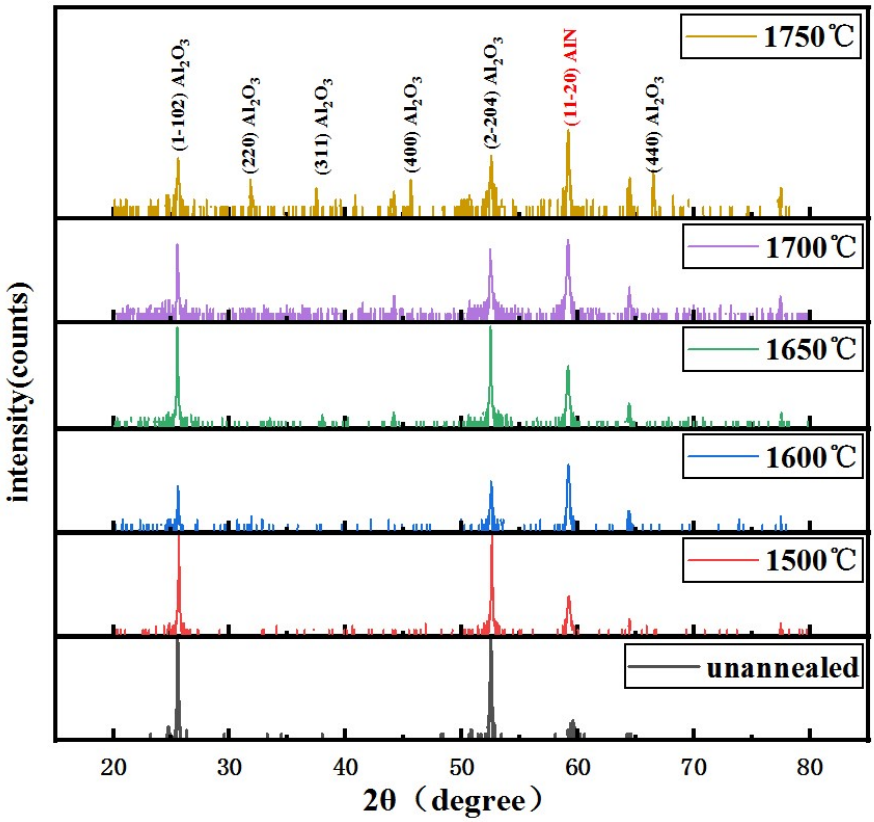


Figure S1. Symmetric ω-2θ XRD scans of AlN layers without and with different annealing temperatures.

**The XRD ϕ scan result of (11-22) plane of a-AlN template without annealing**

To obtain the XRCs of (11-22) plane of a-AlN template, the ϕ scan is the essential step.

However, there is no diffraction peak in the ϕ scan (0-360°) for the (11-22) plane a-AlN without annealing. which is a key step before rocking curve scanning. The result indicates that the intensity of the (11-22) plane XRC of a-AlN template is too weak to be tested, which means the BSFD is too high and the order of the crystal lattice is severely destroyed.

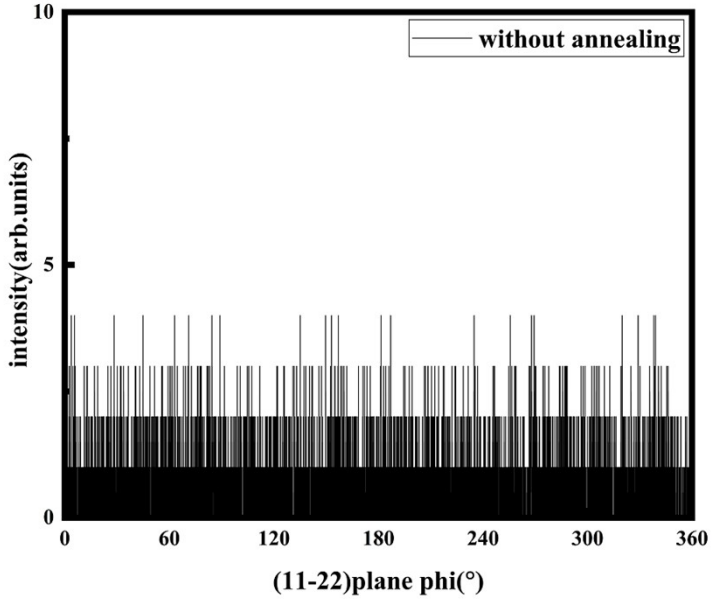


Figure S2. The XRD ϕ scan result of (11-22) plane of a-AlN template without annealing

**W-H plots of a-AlN with different annealing conditions:**

For non-polar nitride films, the modified Williamson-Hall model is widely used as a non-destructive way to measure BSFD.[1] It is estimated by fitting with the FWHM of the XRC diffraction peak of (h0-h0) (h= 1,2,3). The x-ray is incident along the c-axis during the test, which means χ = 30º and ϕ = 0º. The relation used for W-H analysis can be expressed as follows:

$$\Delta\omega_{measure} = \Delta\omega_{mosaic} + \frac{\lambda}{2Lsin\ （\theta_{hkl}）}$$

where $\Delta\omega_{measure}$ is the FWHM of the ω-scan of a reciprocal lattice points hkl, and λ is the wavelength of X-ray source (λ=0.15406 nm), $\theta_{hkl}$ is the Bragg angle for the hkl reflection, $\Delta\omega_{mosaic}$ is tilt angles for the mosaic, L is the LCL (lateral coherence length), and the BSFD of the AlN layer is 1/L. The LCL is extracted from the $y_0$ of the linear fits for the (10-10) and (20-20) diffractions, as shown in Figure S3.

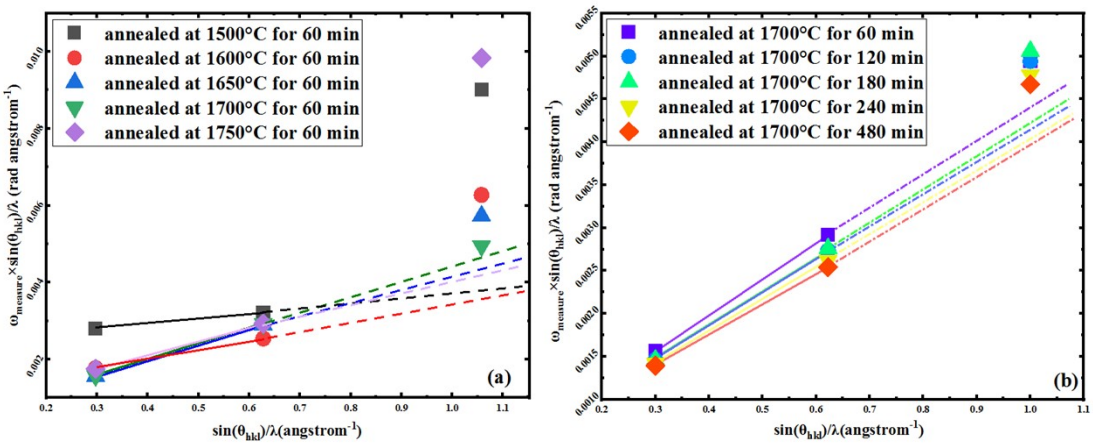


Figure S3 (a)W-H plots of a-AlN films annealed at different temperature for 60 min. (b)W-H plots of a-AlN films annealed a 1700°C for different time.

**The calculation details of the CI-NEB**

In order to explain the mechanism of the decrease of BSFD during HTA process, the first-principles calculations were performed using the projected augmented wave (PAW) plane-wave basis,[2] with an energy cutoff of 400 eV, implemented in the Vienna ab initio simulation package (VASP).[3,4] The generalized gradient approximation (GGA) exchange-correlation DFT functional Perdew-Burke-Ernzerhof (PBE) was employed for the geometrical optimization.[5] The atomic positions were optimized using the conjugate gradient scheme until the maximum force on each atom is less than 0.02 eV/Å. The climbing-image nudged elastic band (CI-NEB) method was employed to locate the transition states during the movement of the stacking fault.[6]

The transition energy barriers are investigated during the elimination of the I1 stacking fault, which has higher percentage in a-AlN.[7] A 2×2×5 supercell of wz-AlN is built, Figure 3 structure A), the atoms follow the stacking sequence of […AaBbAaBb…] (Capital letters correspond to Al, lowercase letter correspond to N) along the [0001] direction, the area along the [0001] direction is 33.91Å$^2$. A 4×4×1 grid is used for the k-point sampling. Based on the wz-AlN, the I1 stacking fault of AlN is built (denoted as 2-layer-I1-AlN, Figure 3 structure I) with the stacking sequence of [...AaBbCcBbCcBbAaBb…] along the [0001] direction. The minimum energy pathway from wz-AlN to 2-layer-I1-AlN is calculated by inserting 19 images between the initial and final state, the energy barrier and atomic structures during the reaction are shown in Figure 3.

**Reference**

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