Local Chemical Origin of Ferroelectric Behavior in Wurtzite Nitrides

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Supplementary information



Figure S1 off axis diffraction analysis for determining in-plane lattice parameter



Figure S2 Definition of chi and omega direction with regard to sample



Figure S3 XRD patterns for various Sc content at thinner region of the library (140 – 150 nm)



Figure S4 (a) Polarization values under each PUND sequence for Al_{0.75}Sc_{0.25}N. Significant
difference between P and U or N and D, which originates from the pure switching current is seen.
The apparent polarization values at U and D come from leakage current and capacitive current.
(b) the current loop under 10 kHz triangle bipolar excitation electric field for Al_{0.75}Sc_{0.25}N. The peaks seen in both polarities represent the switching current.



Figure S5 Al – N bonds in supercell highlighted by bond length ranges. (a) 1.865-1.875 Å, (b) 1.875-1.885 Å, (c) 1.885-1.895 Å, (d) 1.895-1.905 Å, (e) 1.905-1.915 Å, and (f) 1.915-1.925 Å. The shorter length bonds (1.865 – 1.875 Å) are seen on the basal plane Al – N bonds at the same layer of the Sc substitution. The longer length bonds (1.915 – 1.925 Å) are mainly observed in bonds along the polar axis at the same layer of the Sc substitution.



Figure S6 Combinatorial deposition for $Al_{1-x}Sc_xN$ thin film library. (a) schematic diagram of the combinatorial co-sputtering. (b) sputtered film on Pt/TiO_x/SiO₂/Si substrate. The pattern on the film represents gold top electrodes. (c) composition and (d) thickness map in the library.