Epitaxial Growth of High ScN Fraction ScAlN on (111) Si

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ScAlN thin films have attracted significant attention due to their 5× increase in piezoresponse over AlN for $Sc_xAl_{1-x}N$ compositions of $x = 0.43$ [1], leading to applications in 5G filters and RF electronics. Epitaxial growth of ScAlN on Si enables the use of mature MEMS processing technology.

In this work, we demonstrate the growth of $Sc_xAl_{1-x}N$ layers on AlN nucleation layers (NL) on 100-mm (111) Si wafers with x up to 0.40 using MBE. AlN NLs with III/V ratios of 0.5 and 0.8 show polycrystalline ring segments in reflection high-energy electron diffraction (RHEED), III/V of 0.93 gives a streaky RHEED pattern with slight spot-modulation and no apparent etching of the Si substrate, seen in AlN with III/V > 1. Subsequent growth of $Sc_{0.40}Al_{0.60}N$ layers exhibit similar features to the underlying AlN NL, with a single phase wurtzite RHEED pattern only for the AlN III/V = 0.93 sample.

Several ScAlN samples were grown at 410 °C, varying both the Sc and Al flux to allow changes in the III/V ratio for a fixed composition. At low III/V ≤ 0.8, rings appear in the RHEED pattern suggesting the presence of polycrystalline domains. At III/V around 0.95, the ScAlN RHEED is free of extraneous features. At III/V ≥ 1.0 the RHEED pattern broadens and forms indistinct dual-ring-segments. This is the first demonstration of both a lower and upper bound to the high ScN fraction growth space, as well as identification of characteristic RHEED patterns, and is distinct from the III/V ratio behavior at low ScN fraction (x ≤ 0.2).

A graded ScAlN nucleation layer, previously demonstrated for ScAlN/SiC, is further investigated for ScAlN on Si. A 25-nm grade from $x = 0.3 \rightarrow 0.38$ reduces the 0002 X-ray diffraction (XRD) rocking curve full-width at half maximum (FWHM) from 0.90° to 0.73°, and reduces the film stress from 0.92 to 0.59 GPa. Increasing the grade thickness for a fixed total thickness of 133 nm leads to a small reduction in FWHM (0.71°) and stress (0.46 GPa) for a 75 nm grade, with little change for a 115 nm grade.

An optimized ScAlN/AlN/Si sample, having a 10-nm AlN NL, a 20-nm graded 0.32 to 0.40 ScAlN nucleation layer, and a 100-nm $Sc_{0.40}Al_{0.60}N$ layer, shows a clean wurtzite RHEED pattern throughout growth, a FWHM of 1.1°, and an rms roughness of 0.57 nm. Atomic force microscopy height and phase images show no indication of anomalously oriented grains. Such thin, high structural and phase purity films are well suited to high frequency RF MEMS applications.

[1] M. Akiyama, K. Kano, and A. Teshigahara, *Appl. Phys. Lett.,* **95**, 162107 (2009).

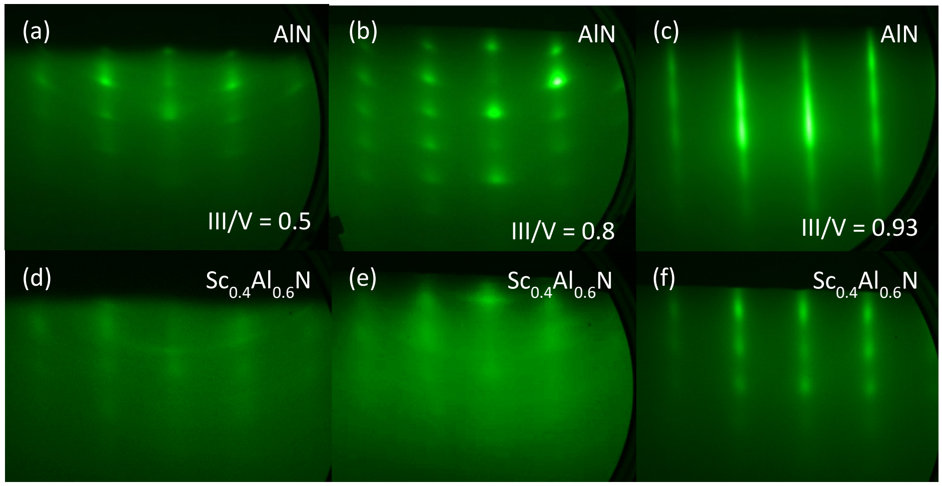

Fig. 1. RHEED images of the AlN nucleation layer and final ScAlN layer, respectively, having III/V ratios of (a,d) 0.5, (b,e) 0.8, and (c,f) 0.93 for 100 nm $Sc_{0.40}Al_{0.60}N$ / 20 nm 0.32 → 0.40 grade / 10 nm AlN / (111) Si samples.

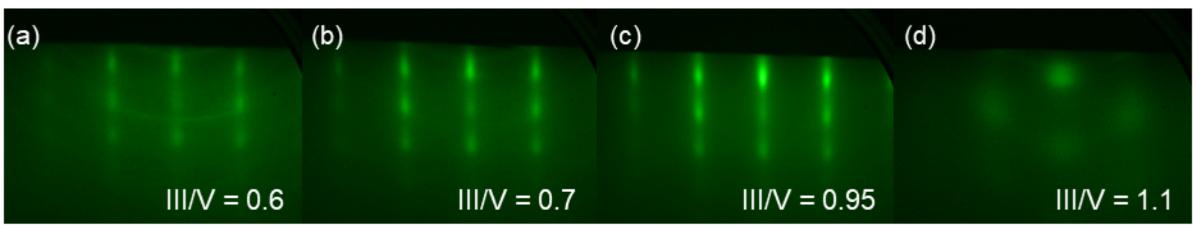

Fig. 2. RHEED patterns showing ScAlN layers grown with varying III/V ratio.

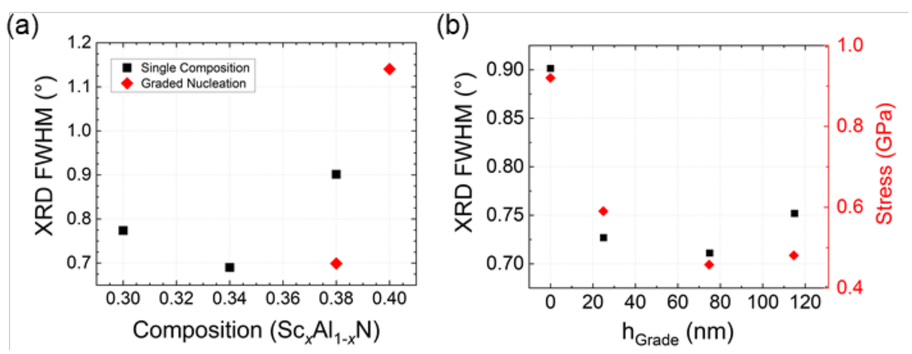

Fig. 3. Dependence of composition and grade thickness on XRD rocking curve FWHM for films with a total thickness (grade plus constant composition) of 133 nm grown on (111) Si.

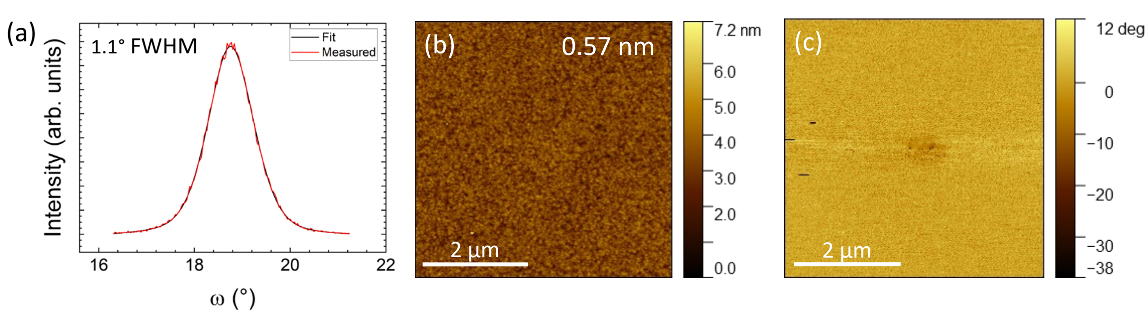

Fig. 4. (a) XRD 0002 rocking curve, AFM (b) height image, and (c) phase image showing an absence of AOGs for 100 nm $Sc_{0.40}Al_{0.60}N$ / 20 nm $Sc_{0.32\rightarrow0.40}AlN$ / 10 nm AlN / (111) Si.