## Kinetically Limited Growth of High Scandium Fraction Scandium Aluminum Nitride

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Thin film AlN-based resonators are the industry standard for microwave-frequency filters used in 4G cell phone technology, and a variety of other RF applications [1].  $Sc_xAl_{1-x}N$  has the potential to replace AlN in next generation devices due a factor of five improvement in piezoelectric response for x = 0.43 [2]. ScAlN is previously been grown by reactive sputtering, which often has relatively high impurity incorporation and high densities of structural defects. Growth of electronic-device-quality ScAlN by molecular beam epitaxy (MBE) has been demonstrated in high-electron-mobility transistor (HEMT) structures using lattice-matched Sc<sub>0.18</sub>Al<sub>0.82</sub>Nbarriers [3]. MBE-growth of high ScN mole fraction ScAlN will enable novel acoustoelectric devices, such as resonant body HEMTs, which take advantage of both the piezoelectric and electronic properties of ScAlN.

200-nm Sc<sub>x</sub>Al<sub>1-x</sub>N samples were grown on 10-nm AlN nucleation layers on 4H-SiC substrates using an RF-plasma MBE equipped with a high temperature effusion cell to supply Sc flux and a dual-filament effusion cell to supply Al flux. Samples with ScN molar fraction varying between 0.10–0.38 were grown at substrate thermocouple temperatures ranging from 400 °C to 920 °C. At moderate ScN fractions of 0.10–0.25, the substrate temperature had minimal impact on ScAlN quality, with films grown at lower temperature having rougher surfaces, but all samples were single-phase wurtzite ScAlN. Reflection high-energy electron diffraction (RHEED) patterns of samples with x = 0.38 grown at 800 °C and 400 °C are shown in Fig. 1, and cross-sectional transmission electron micrographs (TEM) of the same two samples are shown in Fig. 2. The RHEED pattern for the 800 °C-grown sample in Fig. 1(a) shows an extra set of first order spots, consistent with rotated cubic domains, while the TEM image in Fig. 2(a) shows evidence of rock-salt cubic inclusions. However, when grown at 400 °C, both RHEED in Fig. 1(b) and TEM in Fig. 2(b) show single-phase wurtzite ScAlN.

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Figure 1. RHEED images for  $Sc_{0.38}Al_{0.62}N$  samples grown at (a) 800 °C and (b) 400 °C.



Figure 2. TEM images for  $Sc_{0.38}Al_{0.62}N$  samples grown at (a) 800 °C and (b) 400 °C.

## **Supplementary Information**



Figure 3.(a) X-ray diffraction 0002  $2\theta/\omega$  line scan showing a single ScAlN peak and additional weak interference fringes features related to the thin AlN nucleation layer, and (b)  $10\overline{1}5$  reciprocal space map used to calculate the Sc<sub>0.38</sub>Al<sub>0.62</sub>N composition via measurement of the *a*-lattice constant.