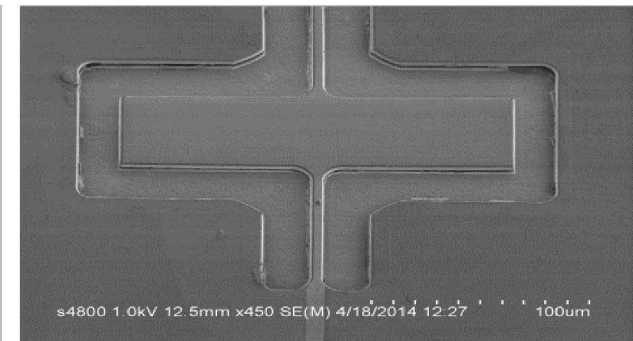
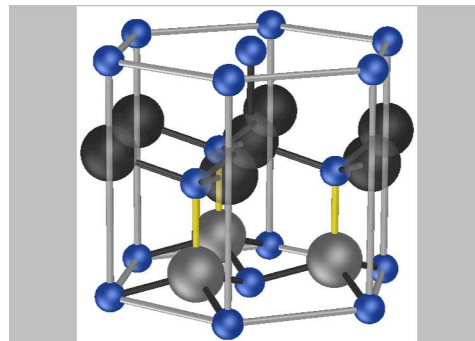
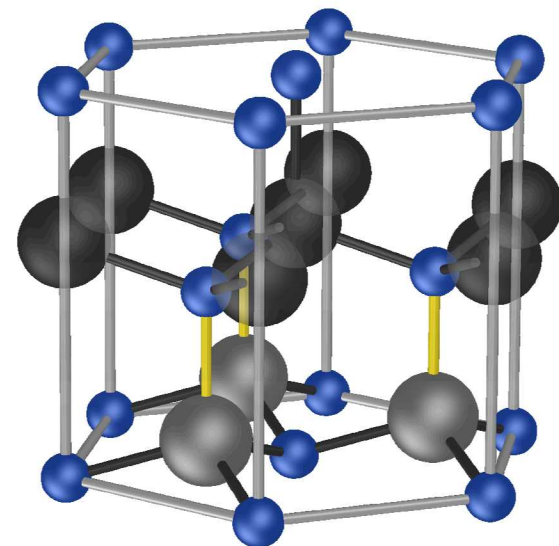




Suppressing Secondary Grains in $\text{Sc}_{0.125}\text{Al}_{0.875}\text{N}$ Using a CMOS Compatible Electrode

Giovanni Esteves, Morgann Berg, Kyle Wrasman, Michael D. Henry,
Benjamin A. Griffin, and Erica A. Douglas

- Piezoelectrics and Aluminum Nitride
- Background and Motivation for $\text{Sc}_x\text{Al}_{1-x}\text{N}$
- Motivation
- Texture Quality of AlN and ScAlN
- Suppressed Secondary Grains in $\text{Sc}_{0.125}\text{Al}_{0.875}\text{N}$
- Conclusion and Acknowledgements



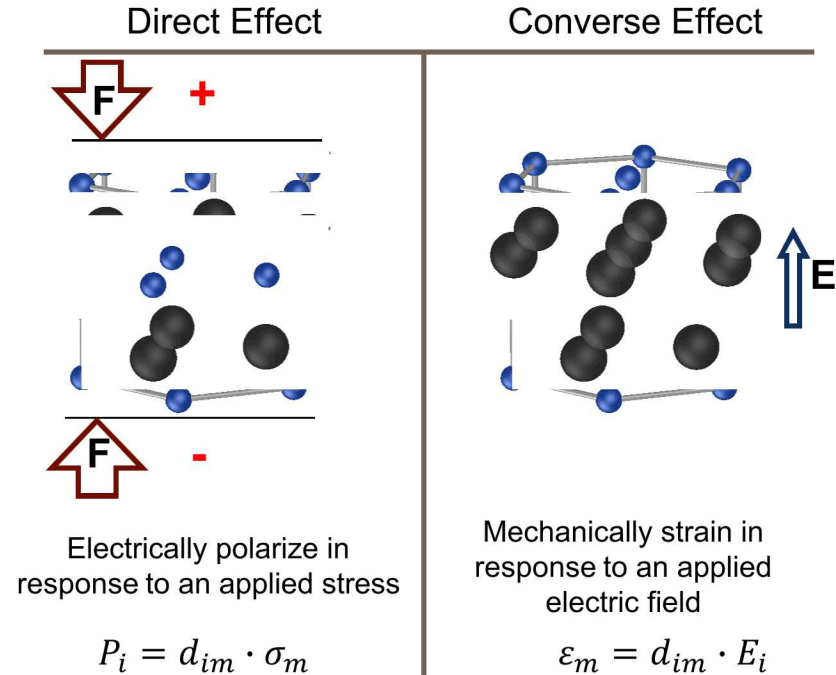
Piezoelectric $\text{Sc}_x\text{Al}_{1-x}\text{N}$

Piezoelectricity

- Material can couple electrical and mechanical energy
 - Direct effect
 - Converse effect
- Magnitude characterized by piezoelectric constant (d_{im})
- Efficiency characterized by electromechanical coupling coefficient (k_t^2)

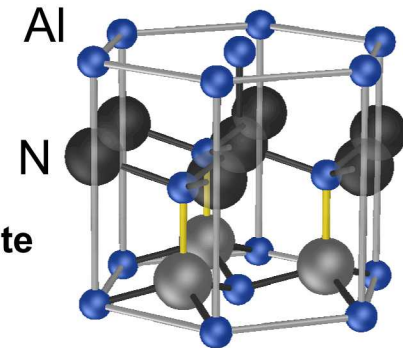
Aluminum Nitride (AlN)

- Reactively sputtered at low deposition temperatures $\sim 350^\circ \text{C}$
- CMOS compatible
- Piezoelectric coefficients
 - $d_{33} = 5 \text{ pC/N}$
 - $d_{31} = -2 \text{ pC/N}$



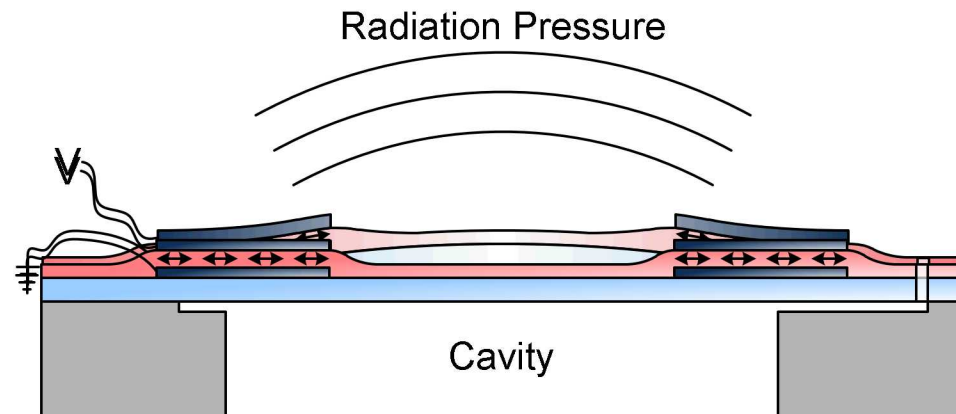
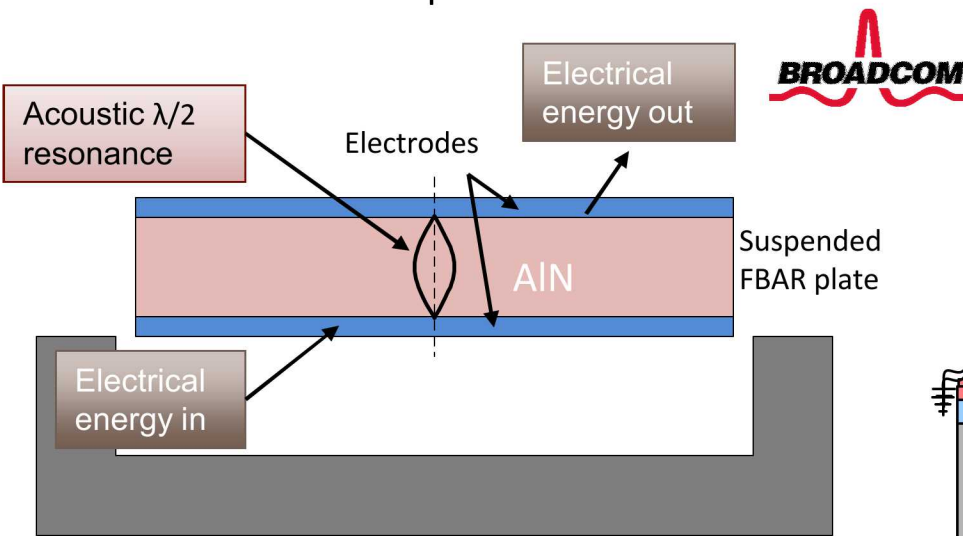
Hexagonal Wurtzite

$$a = 3.11 \text{ \AA}$$
$$c = 5 \text{ \AA}$$



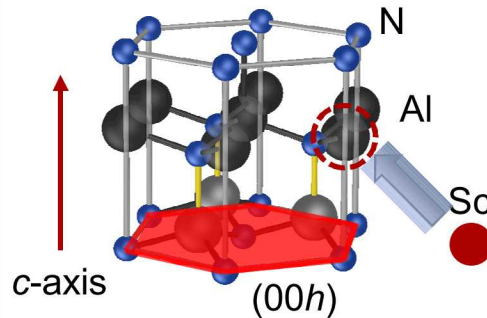
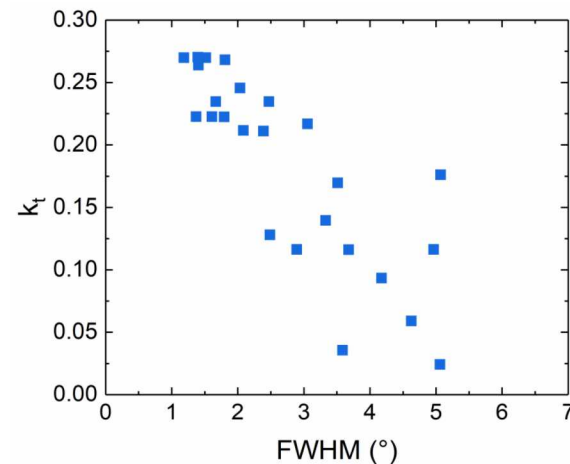
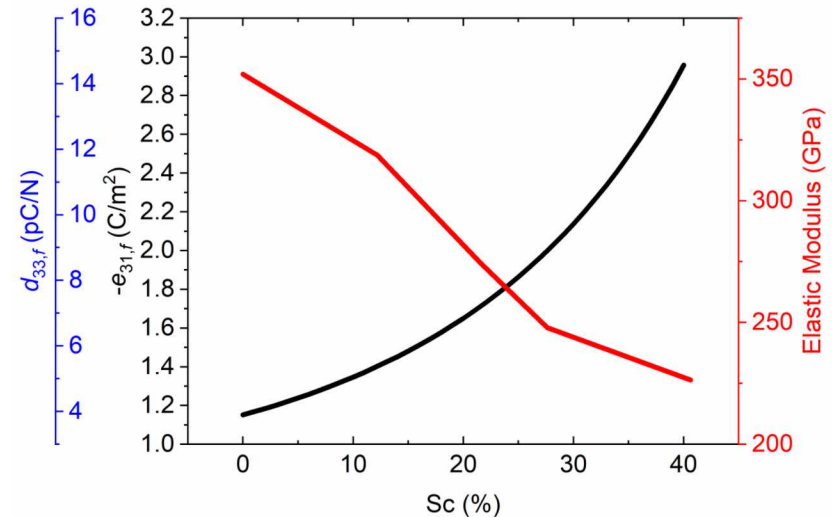
AlN Commercial Success

- Film Bulk Acoustic Resonator (FBAR) Filters
 - Half-wavelength, thickness mode resonators
 - Filter frequency is set by film thickness
 - Commercial success for AlN MEMS
 - >1 billion units produced per year from Broadcom
 - More than 40 discrete filter die in the modern smartphone
- Piezoelectric Micromachined Ultrasonic Transducer (PMUT) Applications
 - Proximity sensing
 - Short range communication
 - Extreme high sound pressure level microphones
 - Imaging
 - Chirp bought by TDK to create devices for gesture recognition



Influence of Sc Alloying in AlN

- $\text{Sc}_x\text{Al}_{1-x}\text{N}$ has the potential to replace current AlN technologies
- Alloying Sc into AlN increases piezoelectric response
- Target orientation for ScAlN is *c*-axis oriented
- Texture quality determined via X-ray diffraction (XRD) rocking curve measurements
 - Full-width half maximum (FWHM) describes how parallel the 002 plane of AlN is oriented with respect to film's surface
- Electromechanical coupling (k_t) increases as texture in AlN films improves

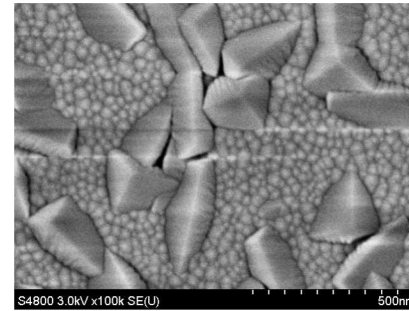


Device Performance Based on Properties

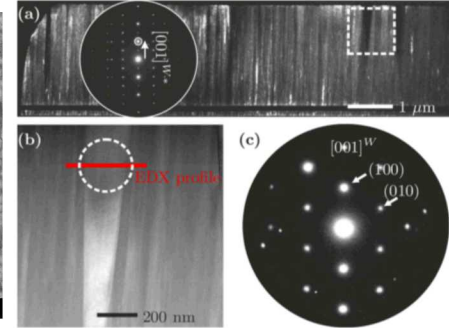
Resonators	$k_t^2 = \frac{e_{31}^2}{E_p \epsilon_{33}}$
Energy harvesting	$FOM = \frac{(e_{31,f})^2}{\epsilon_{33,f}}$
Sensors	$\frac{S}{N} = \frac{e_{31,f}}{\sqrt{\epsilon_0 \epsilon_{33,f} \tan \delta}}$

Challenges with Increasing % Sc and Recent Advances

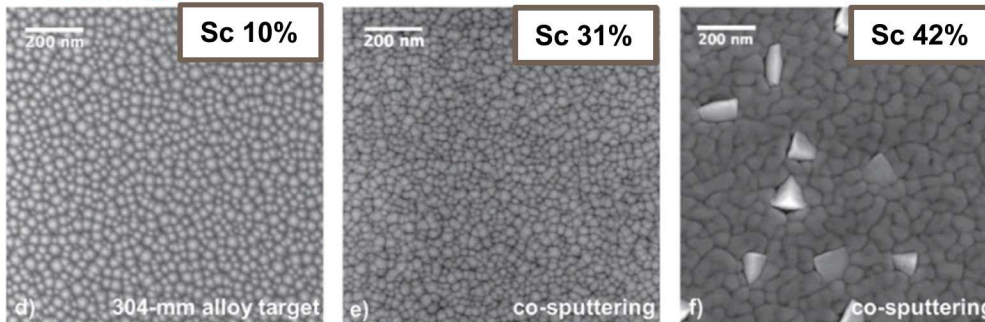
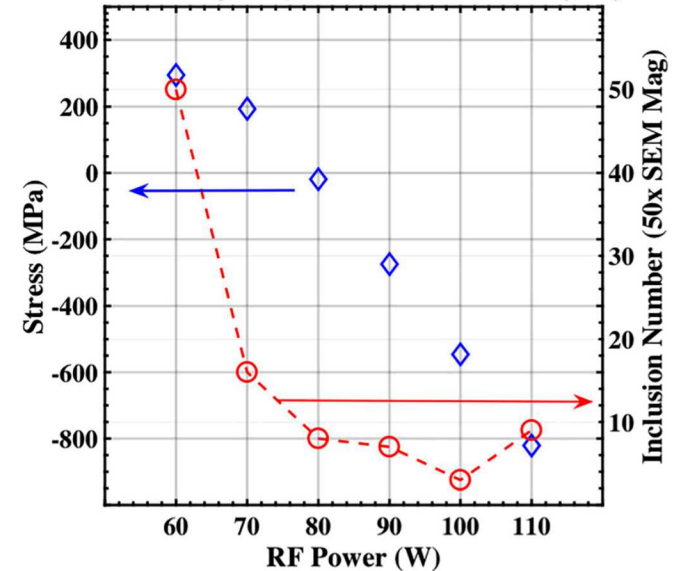
- Secondary grains (SG/inclusions) in ScAlN
 - Increase with Sc concentration
 - Density controlled by processing parameters
- SG have a diffuse {100} orientation
 - Fichtner *et al.*, 2017
- Compressive stress suppresses SG
 - Henry *et al.*, 2018
 - *Compressive stress not optimal for released MEMS*
- Platinum as a bottom electrode on 8" wafers
 - Mertin *et al.*, 2018
 - Significant suppression of SG up to Sc 31%
 - High texture up to 42%
 - *Pt is not CMOS compatible and presents integration challenge*



S. Fichtner *et al.*, *J. Appl. Phys.* 122 (2017)



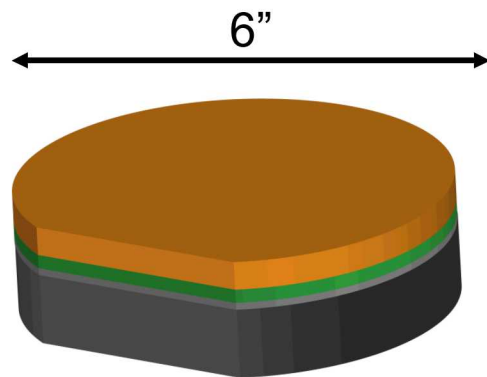
M. D. Henry *et al.*, *J. Vac. Sci. Technol. B* 36 (2018)



- **Motivation:** Need for a CMOS compatible electrode that can achieve highly textured AlN and ScAlN while suppressing secondary grains
 - Alloying Sc into AlN increases the piezoelectric coefficient d_{33} up to **4x** depending on the Sc content
 - $\text{Sc}_x\text{Al}_{1-x}\text{N}$ has the potential for high impact in wireless applications by improving bandwidth and decreasing insertion loss
- **Problem:** The addition of Sc into AlN leads to secondary grains (SG) in the microstructure. Platinum as a bottom electrode can suppress SG but is not CMOS compatible
- **Approach:** Using a stack of Ti/TiN/AlCu to provide similar template to Pt for *c*-axis ScAlN growth with no SG

Metal Stack

- Metal stacks were a combination of Ti, TiN, AlCu (0.5 wt. %)
 - Deposited via physical vapor deposition
 - Titanium deposition used ionized metal plasma (IMP) process for deposition
- Deposited directly onto Si or 1 μm SiO_2



AlN and $\text{Sc}_{12.5}\text{Al}_{87.5}\text{N}$ Films

- Reactively sputtered
 - SPTS Sigma 200 Pulsed DC Magnetron Sputtering System
- 300 mm sputtering target
 - ScAlN films: 12.5% Sc / 87.5% target
 - AlN films: Al target
- Film thickness: 750 nm



Quantifying Texture and Detecting Secondary Grains

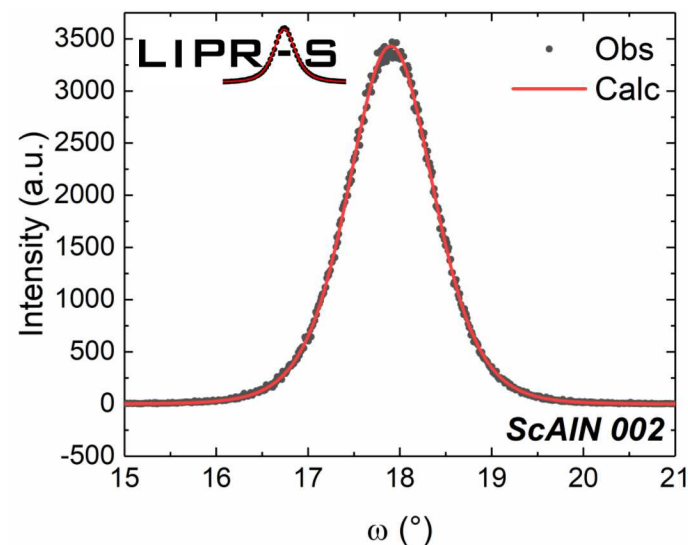
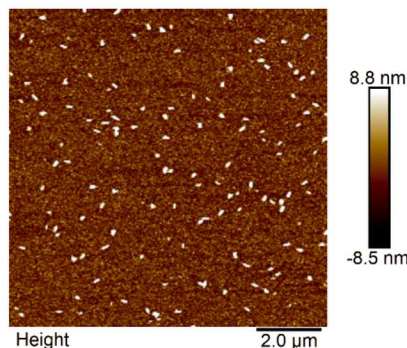
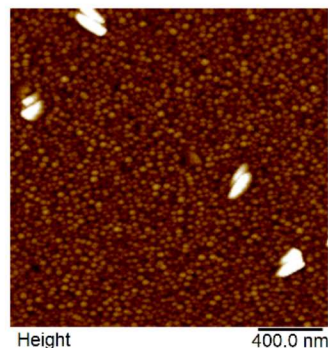
X-ray Diffraction (XRD)

- Texture quality determined via rocking curve measurements
- XRD patterns were measured on a PANalytical X'Pert³ MRD diffractometer
 - Double-bounce monochromator + triple-axis detector
- FWHM from rocking curve measurements extracted through peak fitting



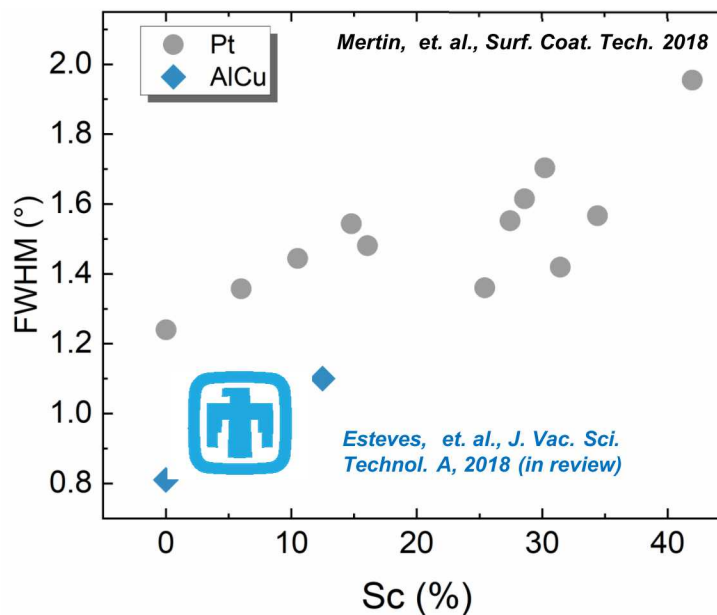
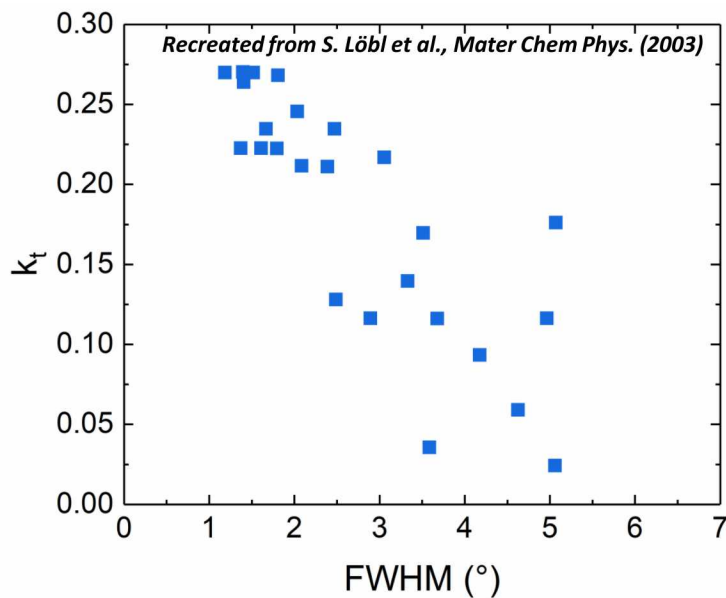
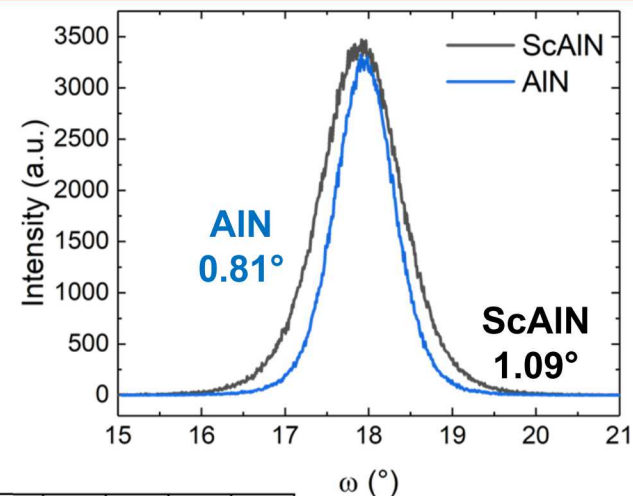
Atomic Force Microscopy and Scanning Electron Microscopy

- Allows for rapid detection of SG
- Yields surface roughness measurements
- NanoScope Analysis software used for data analysis

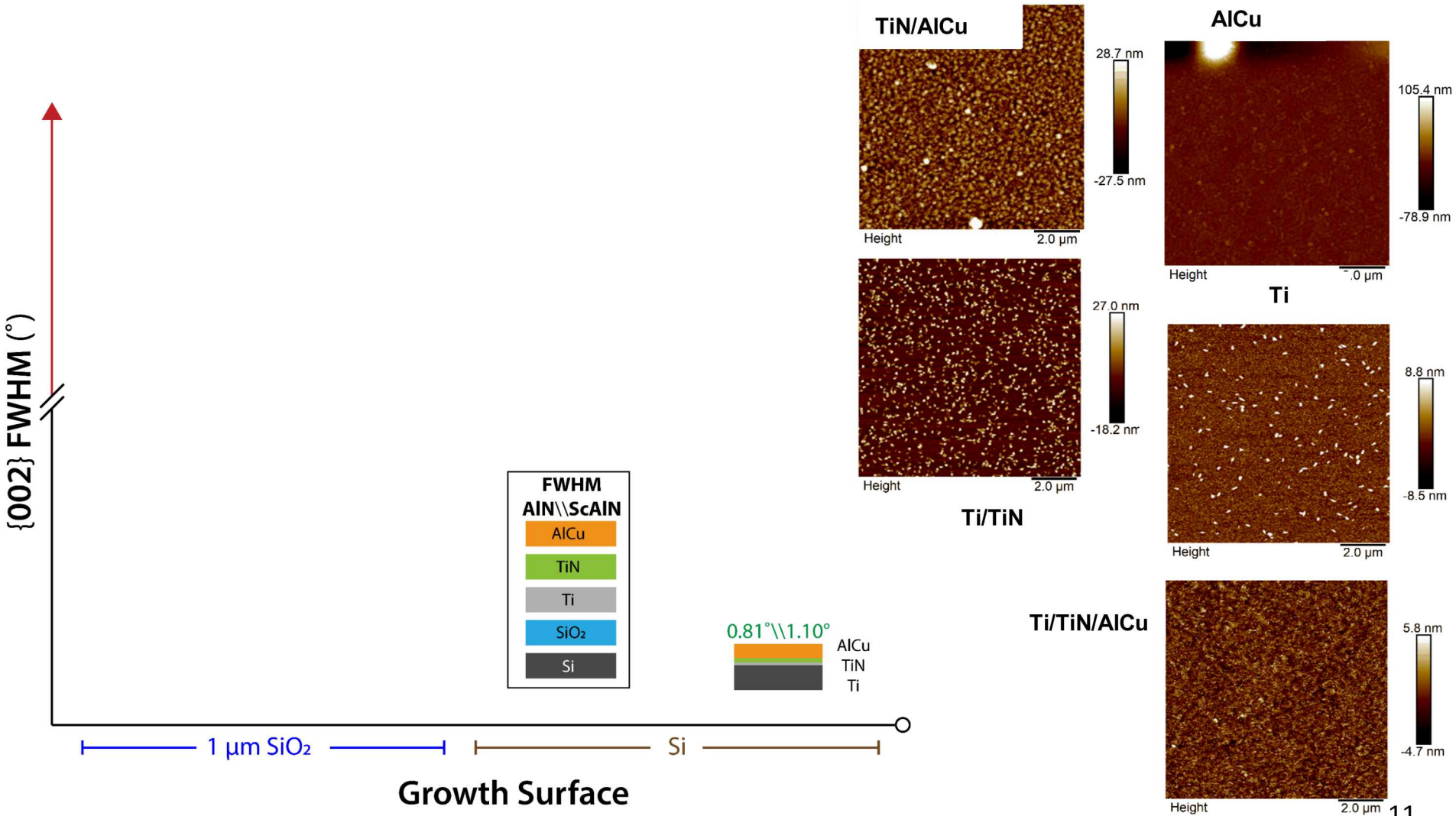


Results: AlN and ScAlN on AlCu

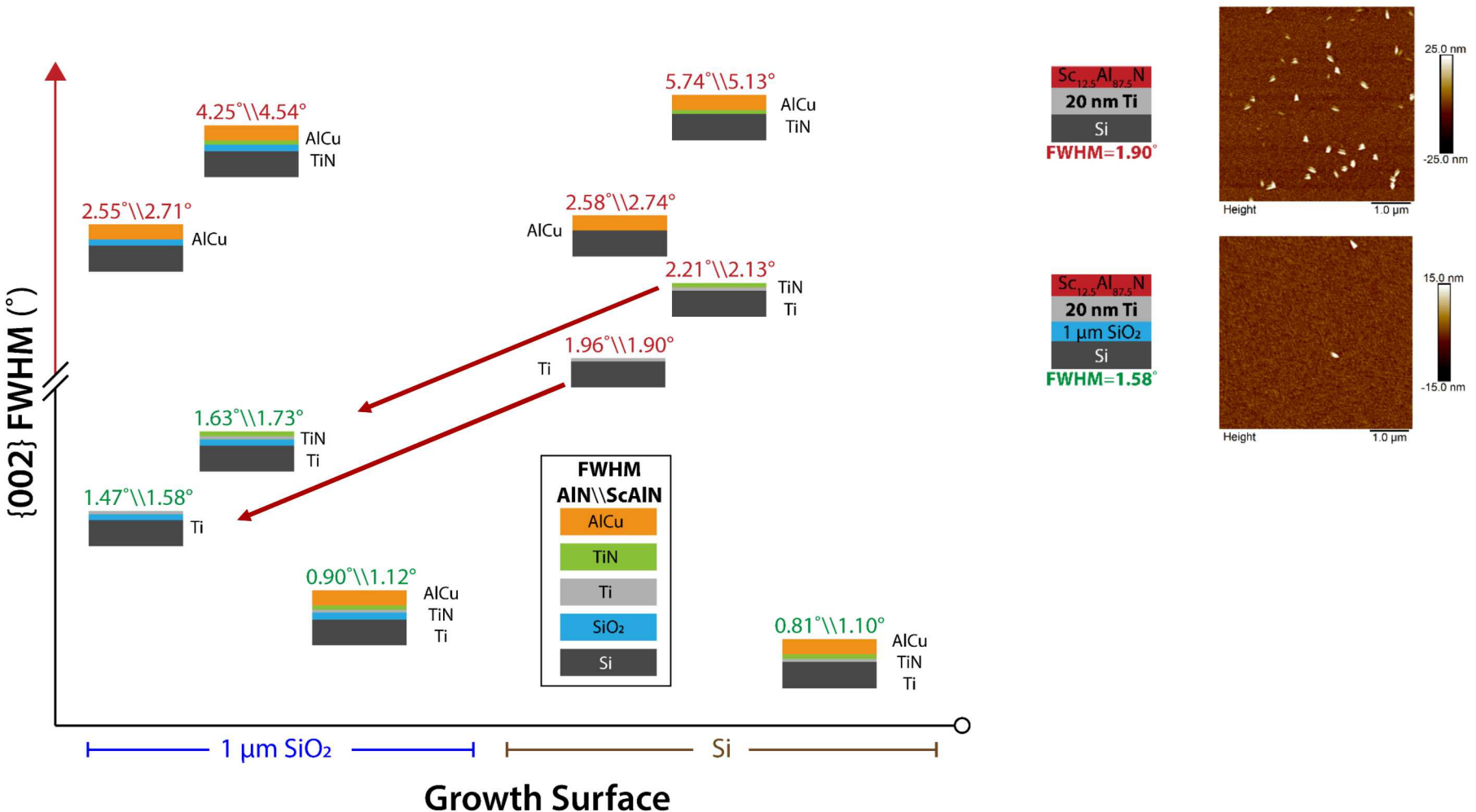
- FWHM of sputtered films on Ti/TiN/AlCu metal stack
 - ScAlN: 1.09°
 - AlN: 0.81°
- Difference between oxide and no oxide underneath metal stack is $< 0.1^\circ$
- Present results are **state-of-the-art** for their given thickness and Sc composition



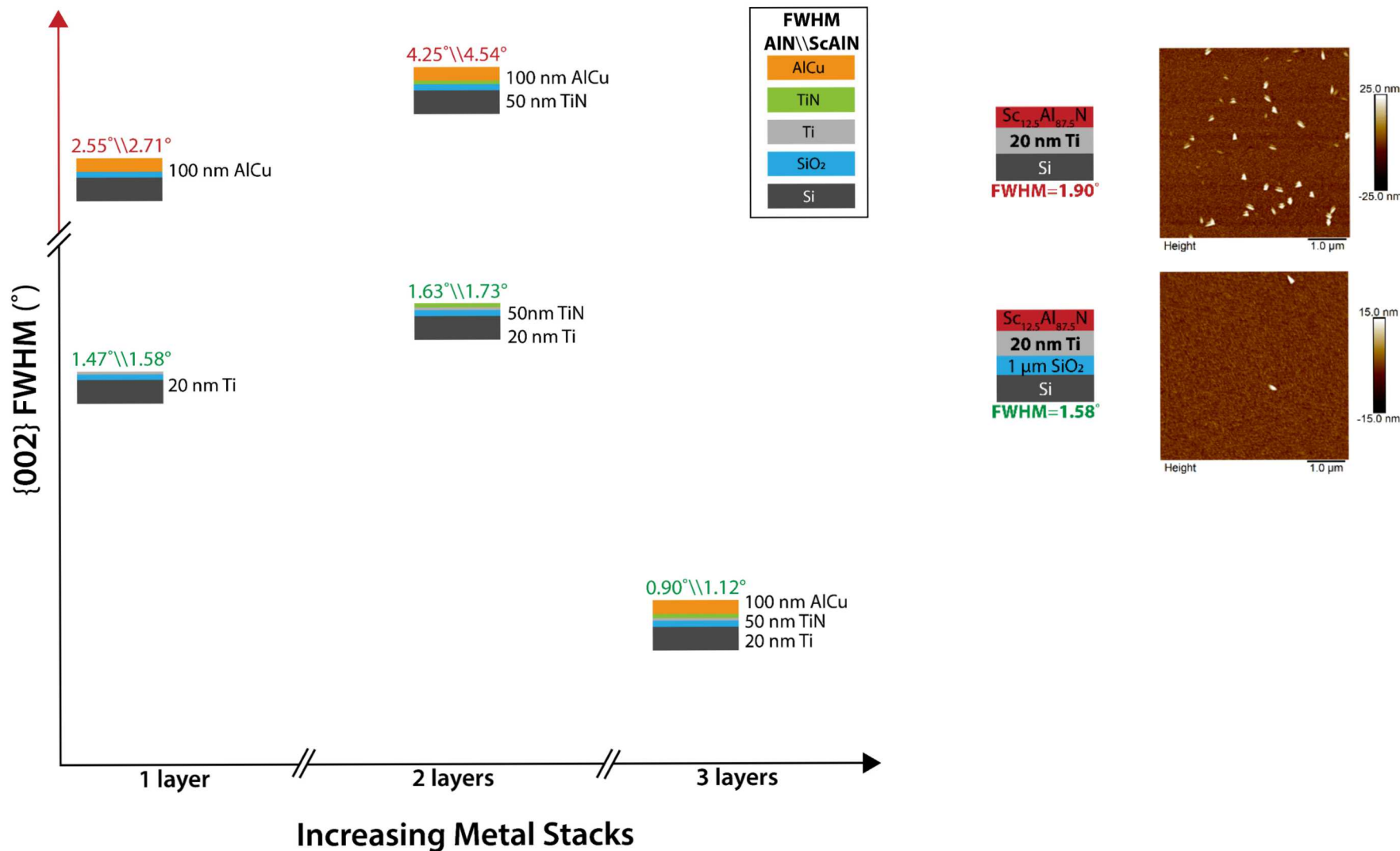
Texture Quality of AlN and ScAlN on Various Metal Stacks



Texture Quality of AlN and ScAlN on Various Metal Stacks



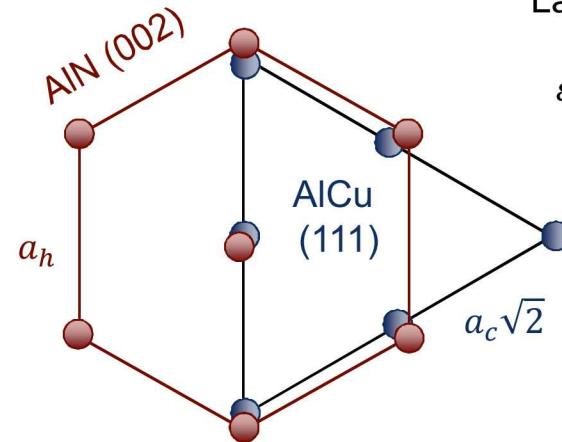
Texture Quality of AlN and ScAlN on Various Metal Stacks



Ti and AlCu as a Bottom Electrode Template

- Face-centered cubic materials show hexagonal symmetry when viewing down the [111]
- Pt and AlCu are both FCC materials but vary slightly in lattice parameter
- Comparing lattice matching between AlCu to AlN and ScAlN
 - 12% for $\text{Sc}_{12.5}\text{Al}_{0.875}\text{N}$
 - 10% for AlN
- Hexagonal {002} Ti has a 5% lattice mismatch to AlN

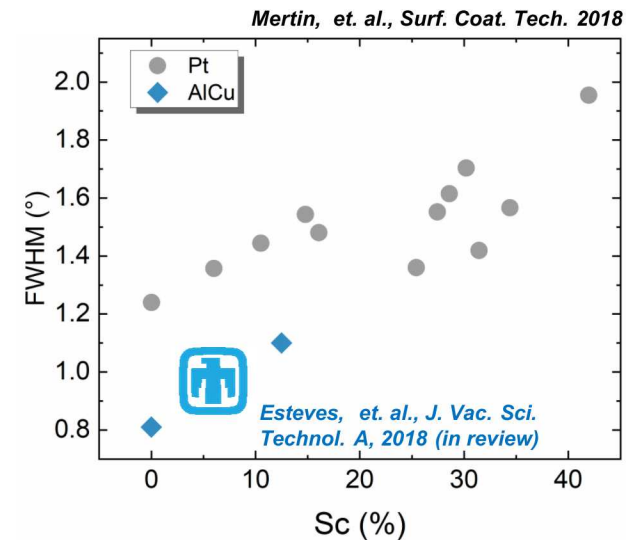
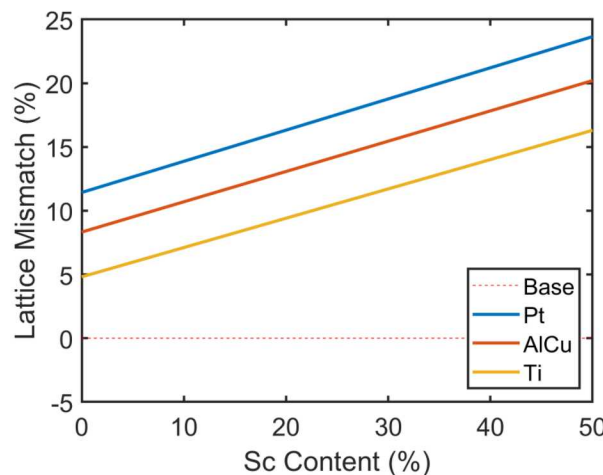
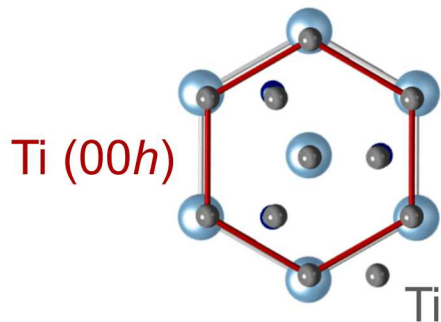
{111} AlCu



Lattice mismatch (ϵ_m)

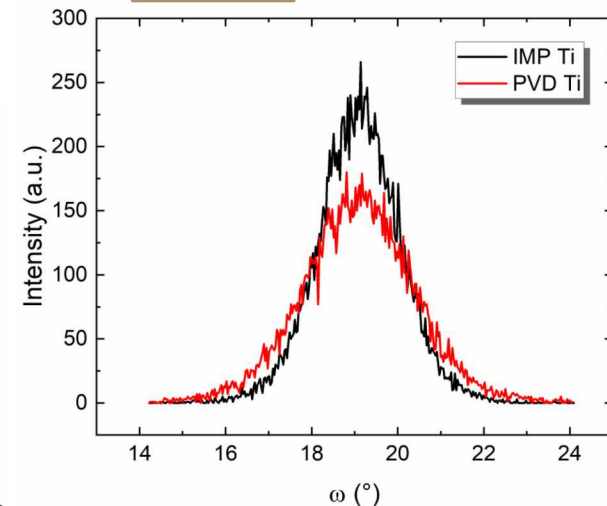
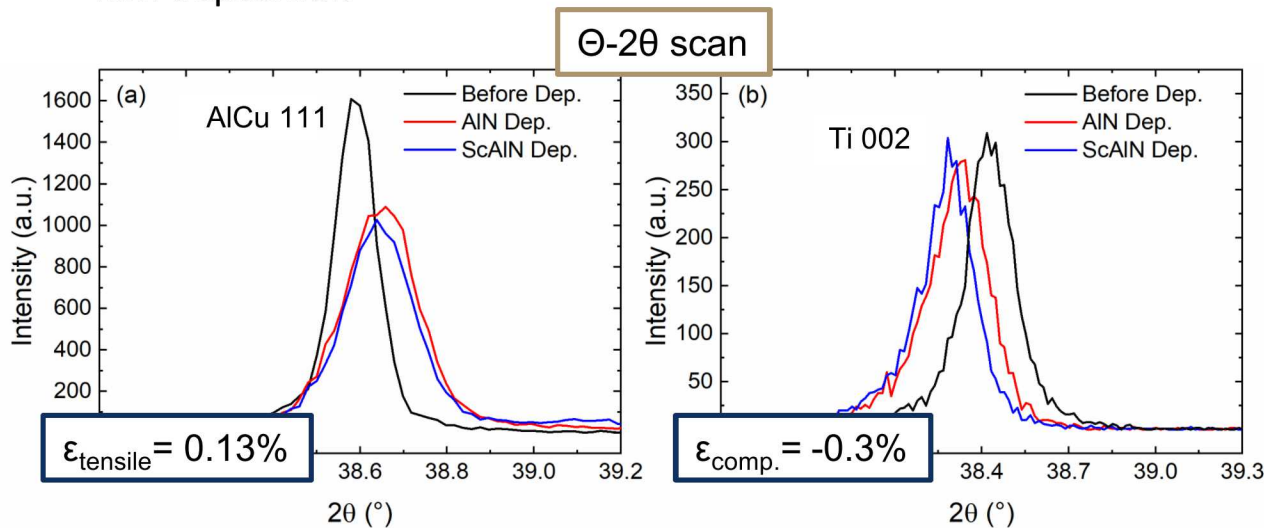
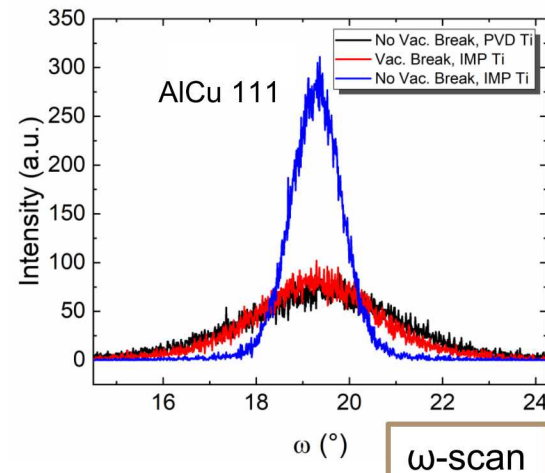
$$\epsilon_m = \frac{2a_h - a_c\sqrt{2}}{a_c\sqrt{2}}$$

Hexagonal {002} Ti



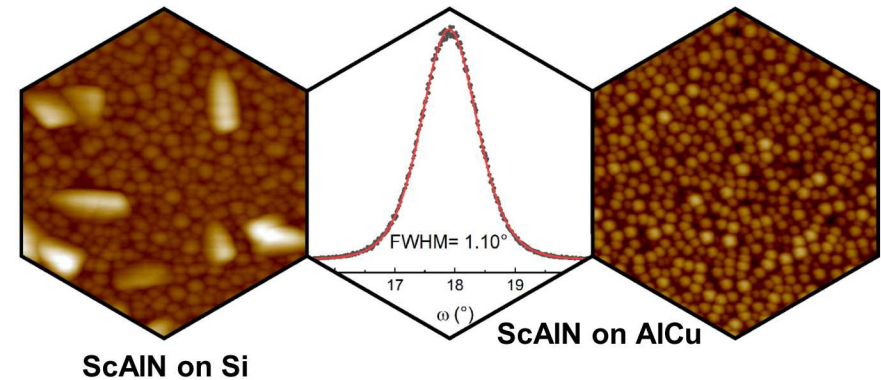
Texture Quality of AlCu and Ti

- Highly textured {111} AlCu is needed to obtain a FWHM of AlN $< 1.0^\circ$
- AlCu texture is very sensitive to processing
 - Growing Ti/TiN/AlCu in same tool
 - Texture of underlying material
 - Method of Ti deposition
 - AlN and ScAlN deposition
- Similar case seen in Ti
- Texture quality improves slightly due to AlN/ScAlN film deposition



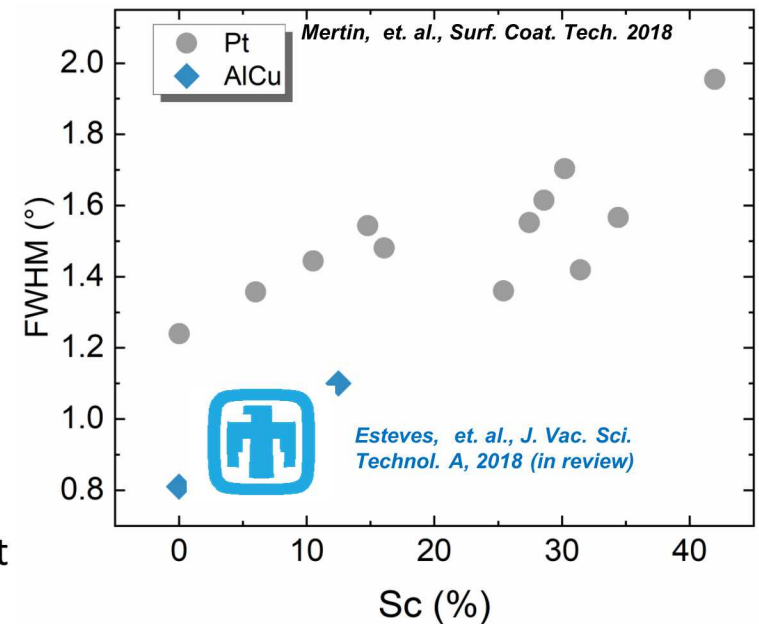
Conclusion and Acknowledgements

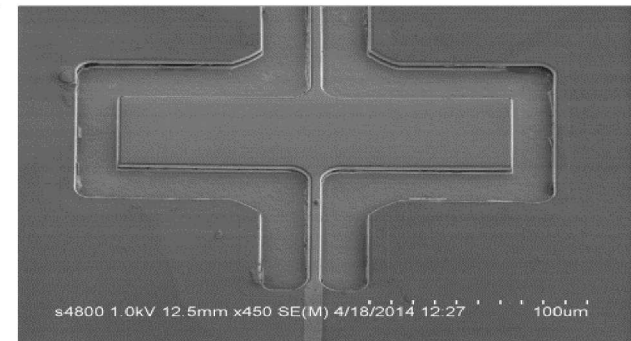
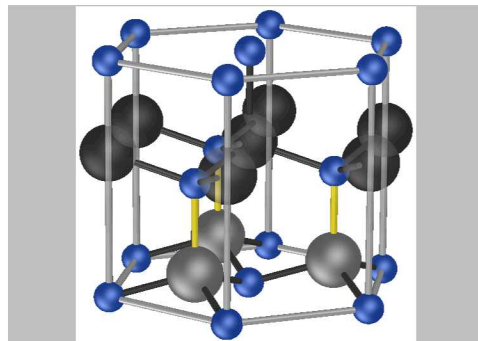
- Ti and AlCu allows for deposition of $\text{Sc}_x\text{Al}_{1-x}\text{N}$ films with a high-quality microstructure and texture up to 12.5% Sc
 - Suppressed secondary grains in ScAlN
 - CMOS compatible metal and allows for commercialization of ScAlN technologies
- TiN is not needed in Ti/TiN/AlCu metal stack to deposit high quality AlN/ScAlN
- Texture of underlying template and its lattice match drive SG suppression



Acknowledgements

- The authors acknowledge and thank the staff of Sandia's MESA fabrication facility for their help in depositing the metal stacks used in this study
- This project was supported by the LDRD program at Sandia National Laboratories





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