Comparing Magnetron Sputtered ScN Films Grown on Sapphire (1 0 -1 0) and (1 -1 0 2) Substrates

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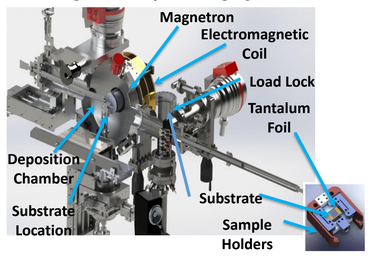
Goal: To understand how growth parameters impact film properties (crystallinity, resistivity, electron density and mobility)

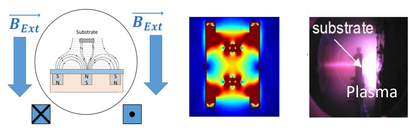
Introduction

- Scandium nitride (ScN) is closely lattice matched to GaN (A semiconductor of interest for high power devices) and serves as a good growth template
- ScN is a thermally and mechanically robust semiconductor (direct bandgap 2.1-2.4 eV) with high electron mobility and low resistivity
- Epitaxial ScN has been grown on sapphire [(0001), (10-10), (1-102)] using MBE, HVPE, and other methods
- Our group has successfully grown epitaxial ScN [(111),(001)] on Sapphire (0001) and MgO (001), respectively, using magnetron sputtering [1]
- The goal of this study is to grow high crystal quality ScN [(002), (022)] films with high electron mobility and low resistivity using a magnetron sputtering system on sapphire [(1-102), (10-10)] substrates, respectively
- To that end, we investigated the impact of various magnetron sputtering growth conditions on the quality of these ScN films. These conditions include substrate temperature, magnetron power, nitrogen fraction and ion flux
- To evaluate the quality of these films, various characterization methods were used, including x-ray diffraction, atomic force microscopy, and Hall effect
- Results from these various characterization methods on the ScN films are presented here

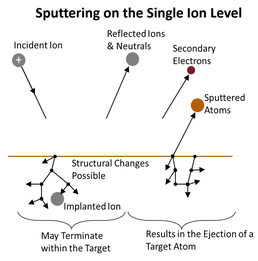
Experimental Setup

Ultra high-vacuum, controllably-unbalanced reactive DC-powered magnetron sputtering system





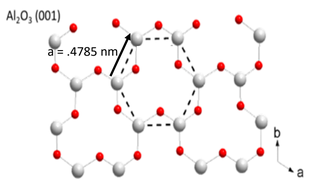
Sputtering on the Single Ion Level



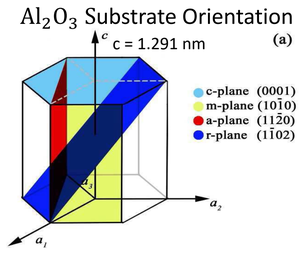
Base Pressure: ~10^{-8} Torr
Growth Pressure: ~20 mTorr
Target to Substrate Distance: ~5 cm

Controlled Growth Parameters
- **Substrate Temperature (500-900°C)**
- **Magnetron Power (50 - 200 W)**
- **Coil Current (0 - 6 A)**
- **N_2 Fraction**

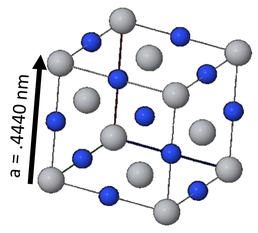
Al_2O_3 Crystal Structure (Wurtzite)



Al_2O_3 Substrate Orientation

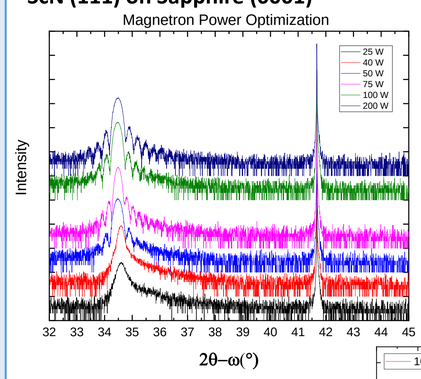


Scandium Nitride Properties:
- Rock salt structure
- Semiconducting:
  Direct band gap = 2.1-2.4 eV
- High carrier concentration:
  10^{19}- 10^{21} cm^{-3}

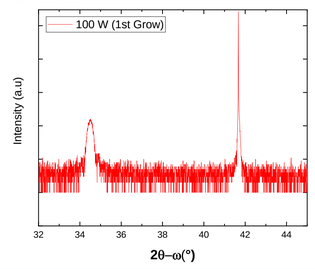


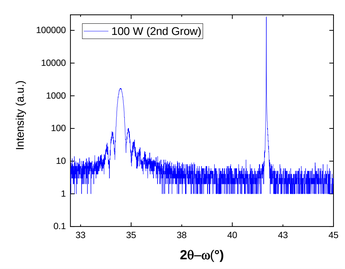
Previous Work: ScN (111) on Sapphire (001) and ScN (001) on MgO (001)

ScN (111) on Sapphire (0001)

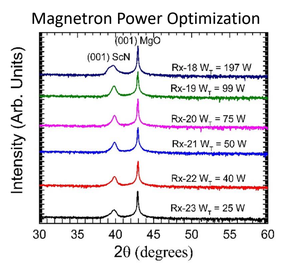


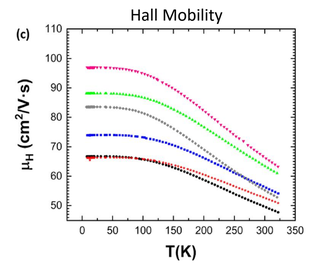
- Note the improvement in crystal quality between the two samples (see below), this change in crystal quality was reflected in almost doubled carrier concentration and increased mobility. (samples grown at nominally same conditions)
- This result indicates an unintentional change in growth parameters, most likely caused by variation in heater resistance
- Room temp. mobility for ScN (111) ranged from 8-14 cm^2/Vs over the tested magnetron power settings

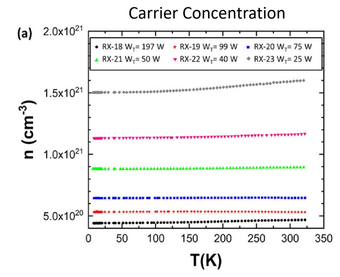




ScN (001) on MgO (001)







Highlights of Previous Studies

- Oxygen and fluorine impurities play a significant role in determining the electrical properties of the ScN films[1]
- For the ScN (002) grown on MgO (001), room temperature mobility was in the range of 66 - 97 cm^2/Vs with carrier concentration on the order of 10^{20} – 10^{21} cm^{-3} [1]

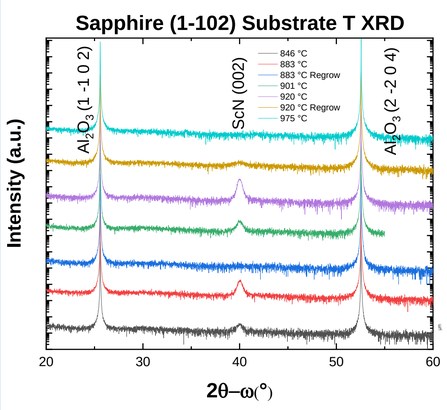
Results

All Samples have nominal thickness of 50 nm

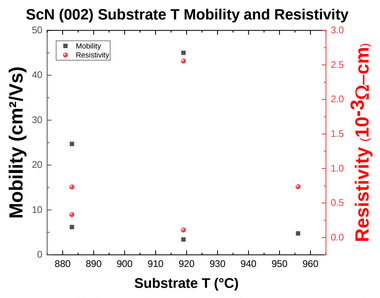
ScN (002), Grown on Sapphire (1 -1 0 2)

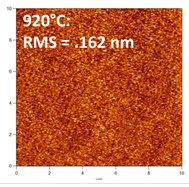
Relaxed d-spacing = .2220 nm

Sapphire (1-102) Substrate T XRD



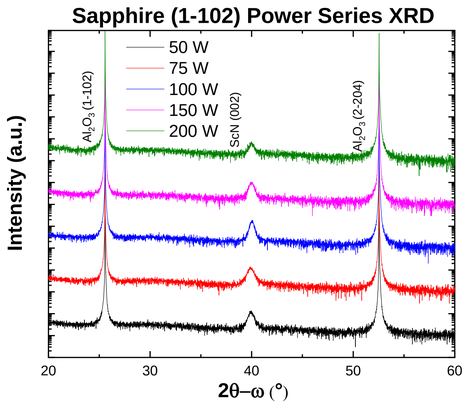
ScN (002) Substrate T Mobility and Resistivity





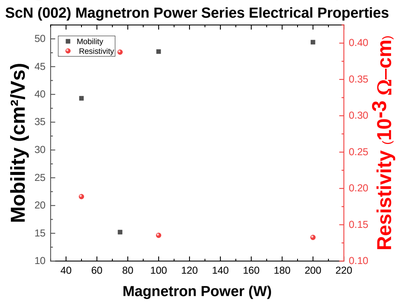
Conditions for the Substrate T series:
Magnetron Power = 100 W
Coil Current = 4 A
Nitrogen Fraction = 75% (15.0 mTorr)

Sapphire (1-102) Power Series XRD



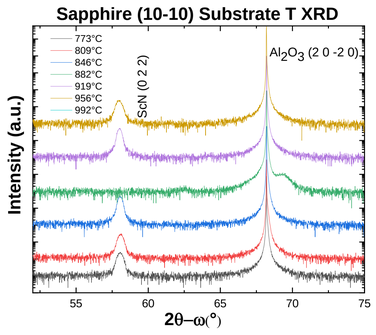
Conditions for the Magnetron Power Series:
Substrate T: 883°C
Coil Current = 4 A
Nitrogen Fraction = 75% (15.0 mTorr)

ScN (002) Magnetron Power Series Electrical Properties

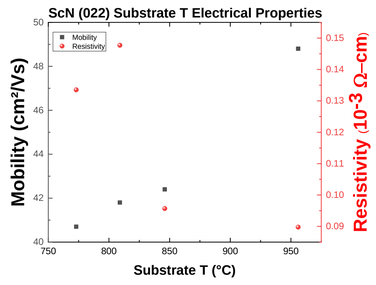


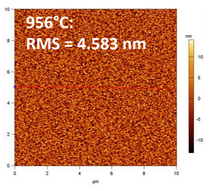
For the Substrate T series:
Magnetron Power = 100 W
Coil Current = 4 A
Nitrogen Fraction = 75% (15.0 mTorr)

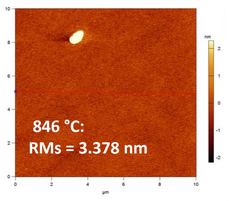
Sapphire (10-10) Substrate T XRD



ScN (022) Substrate T Electrical Properties



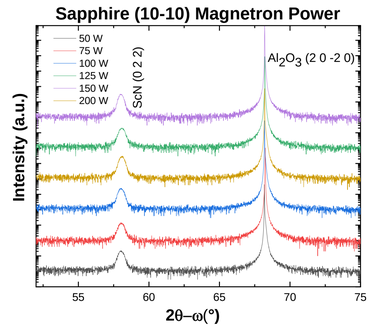




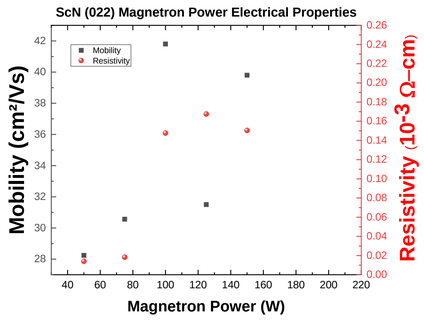
ScN (022), Grown on Sapphire (1 0 -1 0)

Relaxed d-spacing = .2029 nm

Sapphire (10-10) Magnetron Power



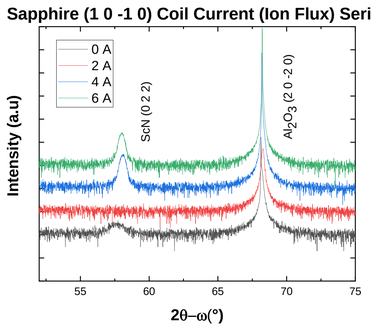
ScN (022) Magnetron Power Electrical Properties



Conditions for the Magnetron Power Series:
Substrate T: 809°C
Coil Current = 4 A
Nitrogen Fraction = 75% (15.0 mTorr)

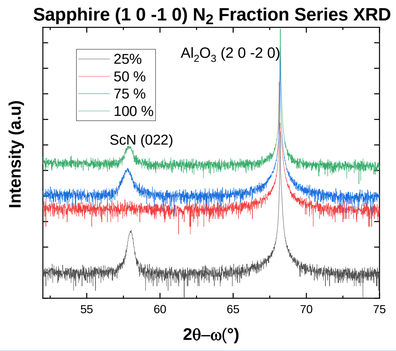
Conditions for the coil current series:
Substrate T: 809°C
Magnetron Power: 100 W
Nitrogen Fraction = 75% (15.0 mTorr)

Sapphire (1 0 -1 0) Coil Current (Ion Flux) Series



Conditions for the nitrogen fraction series:
Substrate T: 809°C
Coil Current = 4 A
Magnetron Power: 100 W

Sapphire (1 0 -1 0) N_2 Fraction Series XRD



Summary of Study

- The crystalline quality of the grown films is not as of high quality as that of ScN (111).
- Current results indicate (022) ScN is of better quality than (002) ScN based on XRD.
- Substrate temperature is much more important for the (002) ScN than the (022) films.
- The results of our N_2 fraction study indicate that optimal growth conditions for (002) require a lower N_2 fraction than that of (111) ScN.
- The mobility of all measured samples, regardless of the orientation, is lower than that of ScN films grown on MgO (001), but mobility is higher than that of the ScN (111).

Future Work

- Continue N_2-fraction study for (1 0 -1 0) orientation and initiate this study for the (1 -1 0 2)
- Revisit samples showing atypical crystalline or electrical results
- Expand XRD scans to determine crystal structure
- Initiate XPS to better understand composition (impurities significantly impact electrical properties)
- Additional Hall effect measurements of ScN (002) and (022)

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References

1. Electronic transport in degenerate (100) scandium nitride thin films on magnesium oxide substrates ,Appl. Phys. Lett. 113, 192104 (2018); https://doi.org/10.1063/1.5050200
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