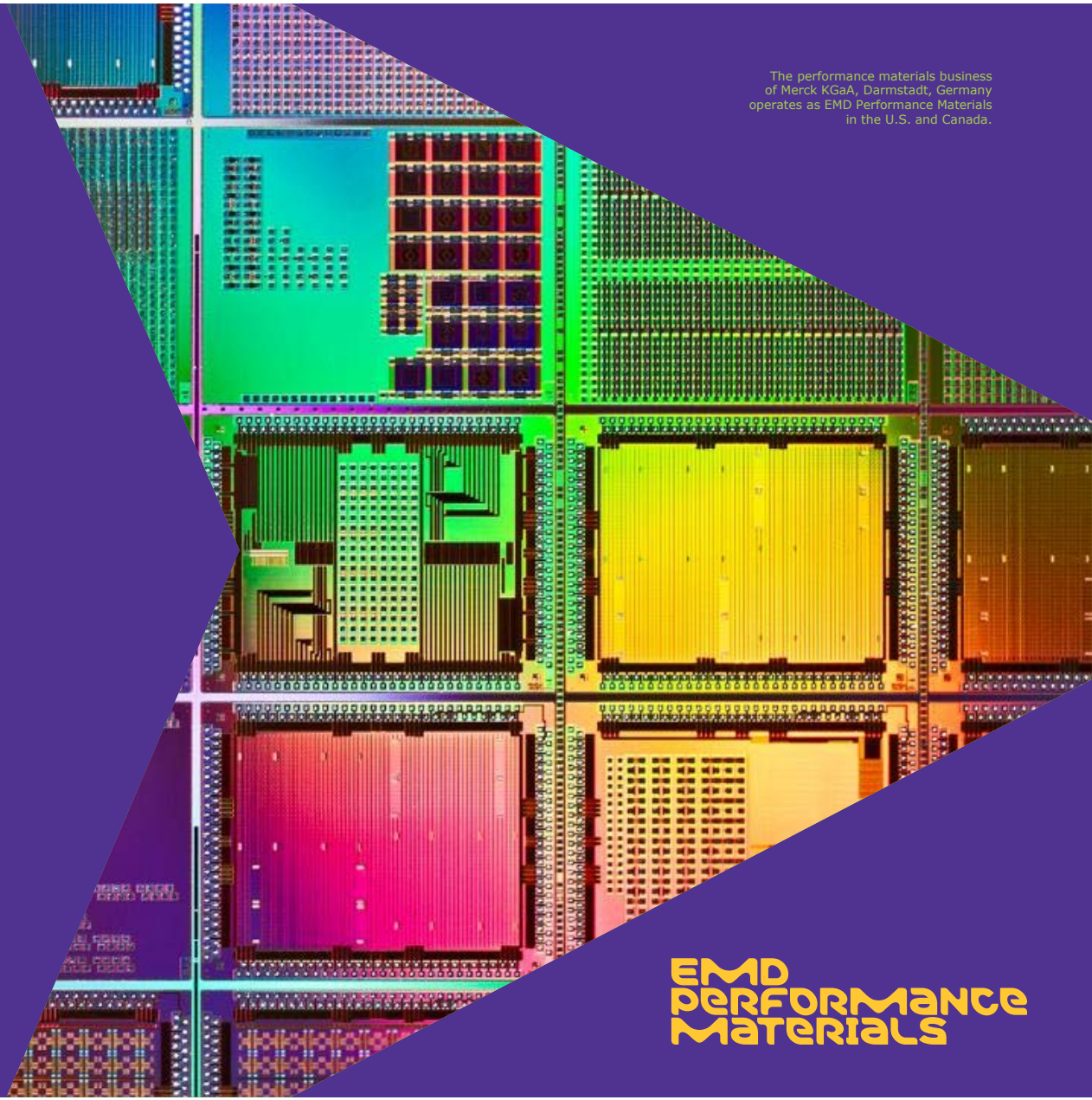
Atomic layer deposition of niobium nitride thin film with $NbCl_5$ and NH_3

Moo-Sung Kim[1], Se-Won Lee[1], and Sergei Ivanov[2]



EMD PERFORMANCE MATERIALS

Atomic Layer Deposition of Niobium Nitride
Motivation

Key Properties

- Thermodynamically stable toward Cu
- High melting point
- Chemically inert
- Good mechanical properties, such as hardness and toughness
- Low resistivity, good adhesion
- Lower work function compared to TiN

Potential Applications

- Barrier layer
- Metal gate
- Electrode material

Project goals

- Study ALD of NbN on various substrates
- Confirm good process conformality

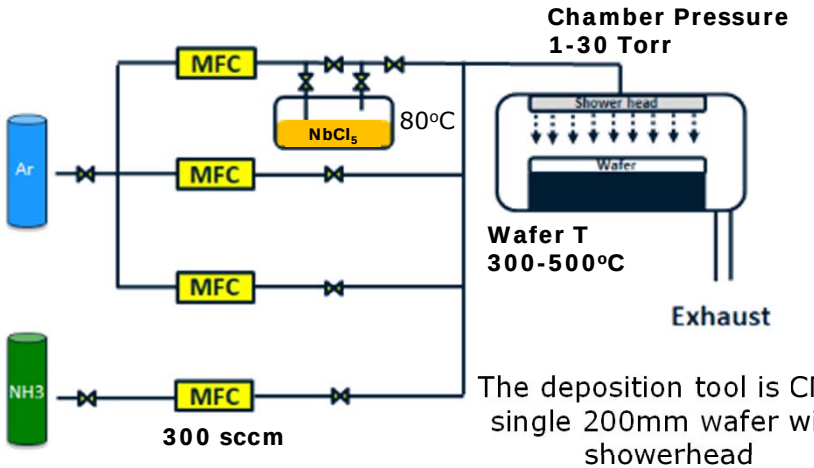
Metal Nitride	Work Function, eV
TiN	5.05 – 5.15
VN	5.05 – 5.15
NbN	**4.95**
HfN	4.70 – 4.80
TaN	4.70 – 4.80

R. Fujii et al, Vacuum, 2006, 80, p. 832-835

Atomic Layer Deposition of Niobium Nitride
ALD precursor and ALD tool

- Niobium pentachloride, $NbCl_5$, was evaluated as a potential precursor for the deposition of NbNx films
- Deposition on Si, SiO_2, Al_2O_3 and TiN substrates was investigated
- The impact of chamber pressure and wafer temperature on ALD process was studied

Tool Configuration



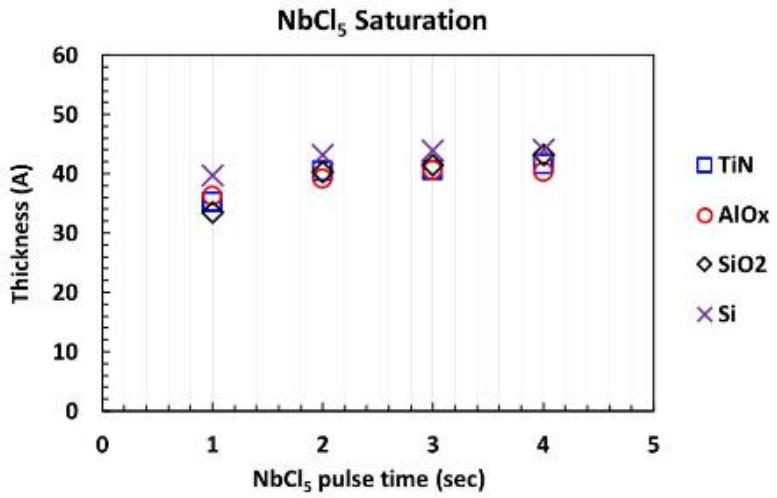
The deposition tool is CN-1 single 200mm wafer with showerhead

NbN_x Film Characterization

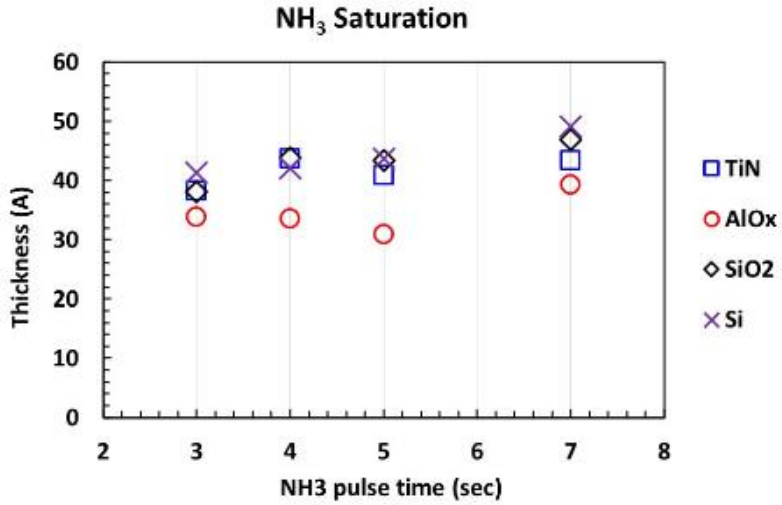
- Thickness and Resistivity: XRF, 4 point probe
- Film Composition: RBS, XPS, SIMS
- Film properties: XRR and XRD
- Surface morphology and Conformality: SEM & TEM

Atomic Layer Deposition of Niobium Nitride
Saturation Behavior at 350°C and 20 torr

- $NbCl_5$ showed good saturation behavior independent of substrate
- More variability was observed during ammonia saturation study on AlOx
- 3/30/5/30 was used as a reference recipe for film saturation



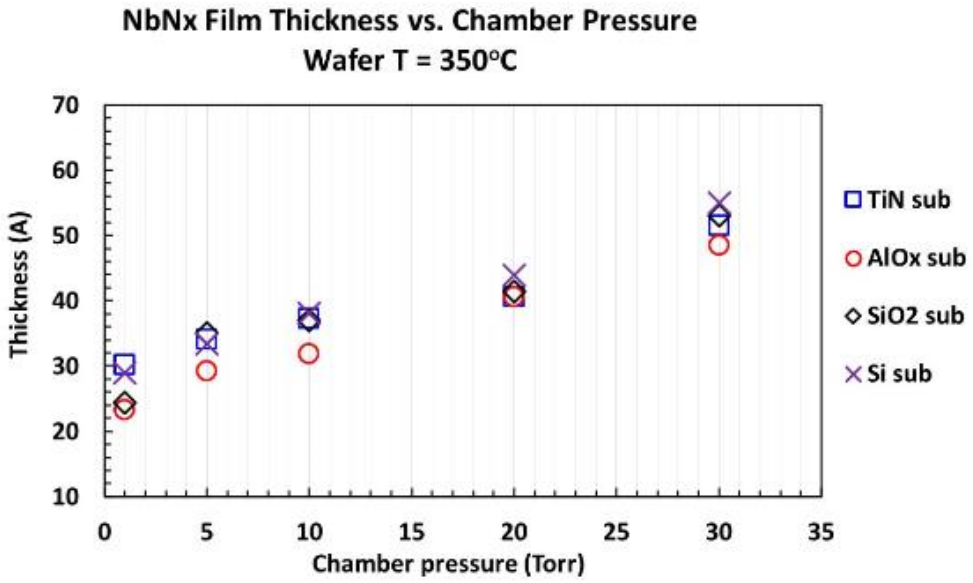
$NbCl_5/Ar/NH_3/Ar$ = x/30/5/30 x100 cycles



$NbCl_5/Ar/NH_3/Ar$ = 3/30/x/30 x100 cycles

Atomic Layer Deposition of Niobium Nitride
The Impact of Chamber Pressure on Growth Rate

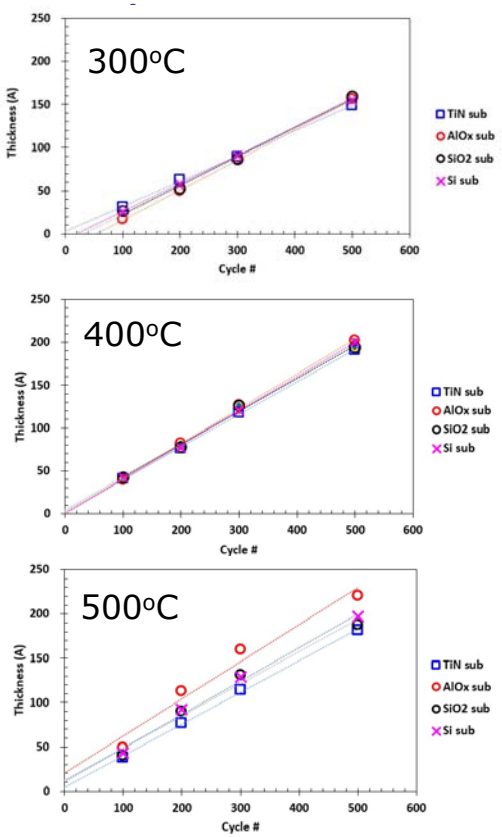
- Deposition rate increased with increase in chamber pressure
- No significant impact of substrate on film thickness



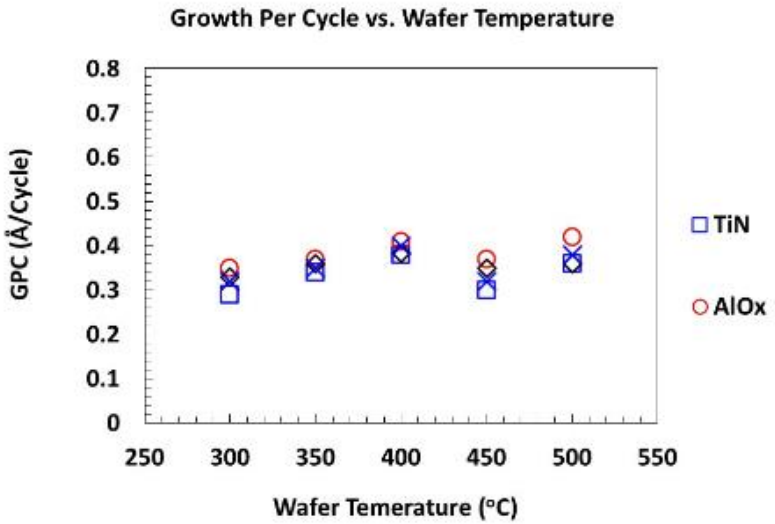
$NbCl_5/Ar/NH_3/Ar$ = 3/30/5/30 x100 cycles

Atomic Layer Deposition of Niobium Nitride
GPC and Wafer Temperature Dependence at 10 torr

NbNx Film Thickness vs. Cycle # at Different Wafer Temperatures

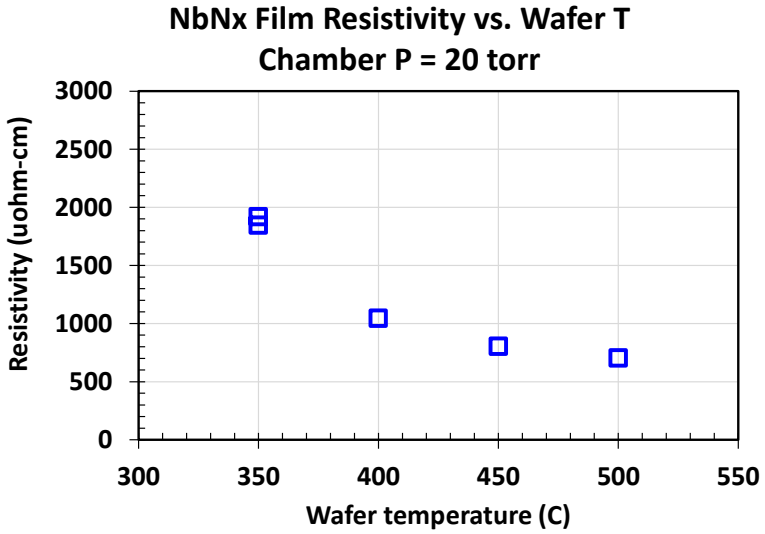


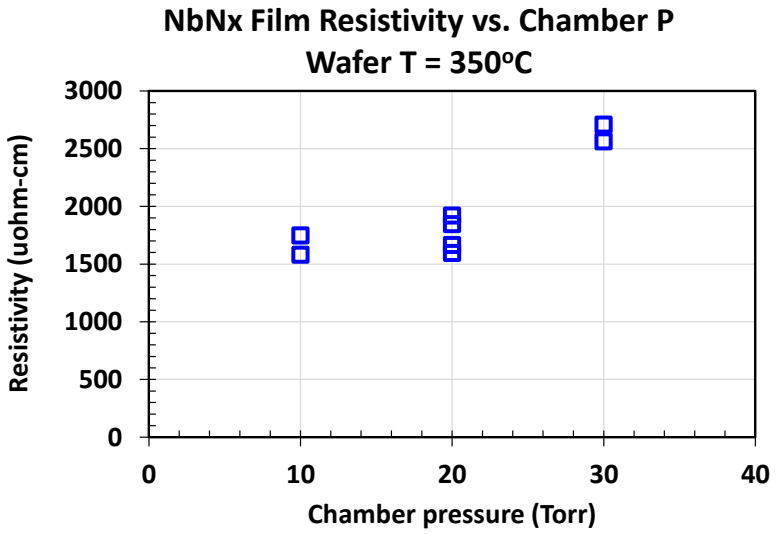
- No nucleation delay and good linearity observed up to ~ 450°C
- Above 450°C more variation between substrates was observed, likely due to minor reactivity of $NbCl_5$ with substrates



Characterization of Niobium Nitride Film
Film Resistivity

- Resistivity of NbNx film decreased gradually as the deposition temperature increased. The resistivity at 350°C was ~ 1,900 uohm-cm, whereas it was ~700 uohm-cm at 500°C
- No improvement in film resistivity with increase in chamber pressure was observed

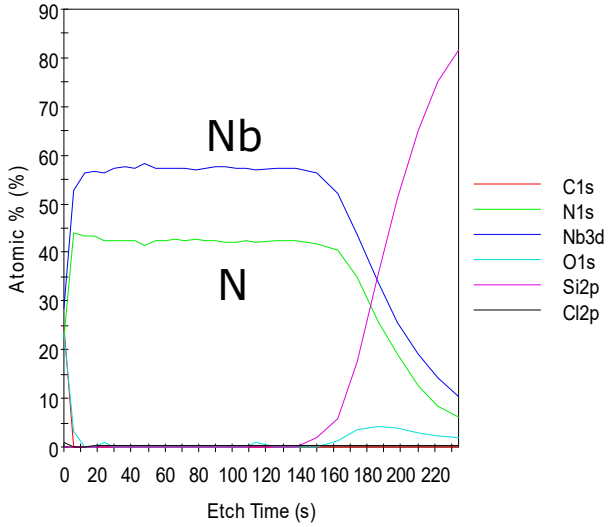




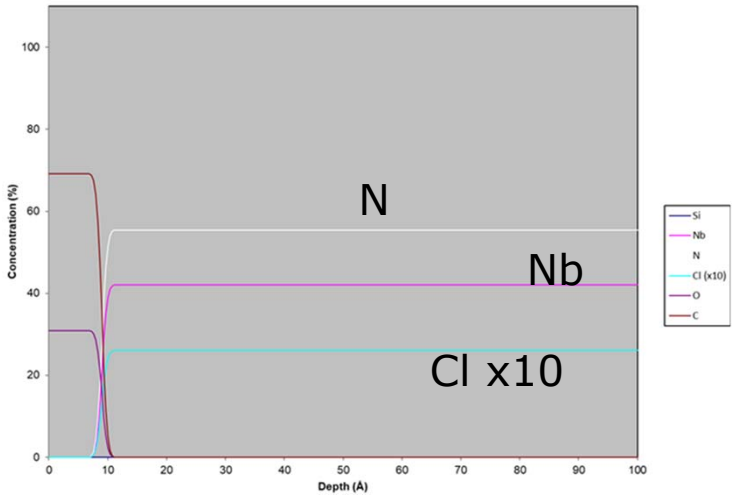
Characterization of Niobium Nitride Film
XPS and RBS Analysis

- Discrepancy between XPS and RBS analysis was observed at all testing conditions
- XPS profile showed Nb-rich films, likely due to preferential sputtering of nitrogen
- RBS profile showed N-rich film, more consistent with Nb_4N_5 structure
- XRD and SIMS analyses were also conducted to confirm film composition

XPS Profile of NbNx deposited at 350˚C

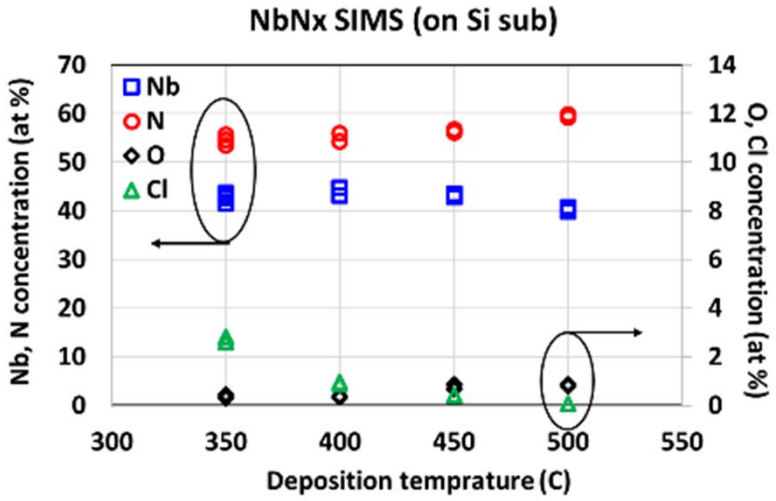


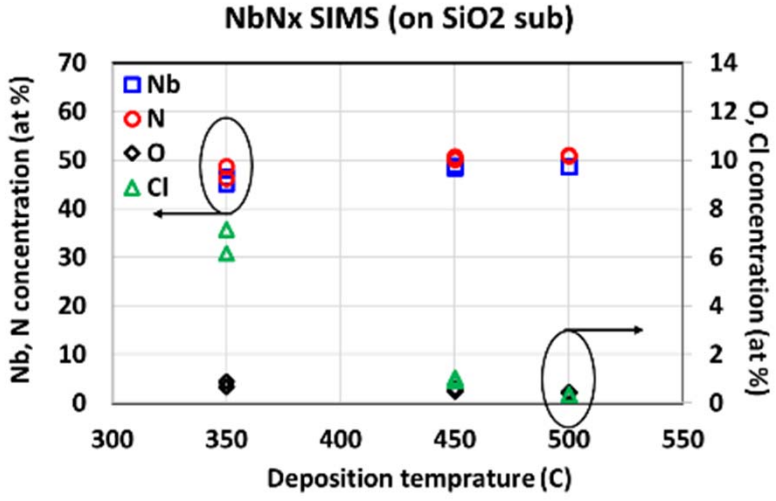
RBS Profile of NbNx deposited at 350˚C



Characterization of Niobium Nitride Film
SIMS Analysis

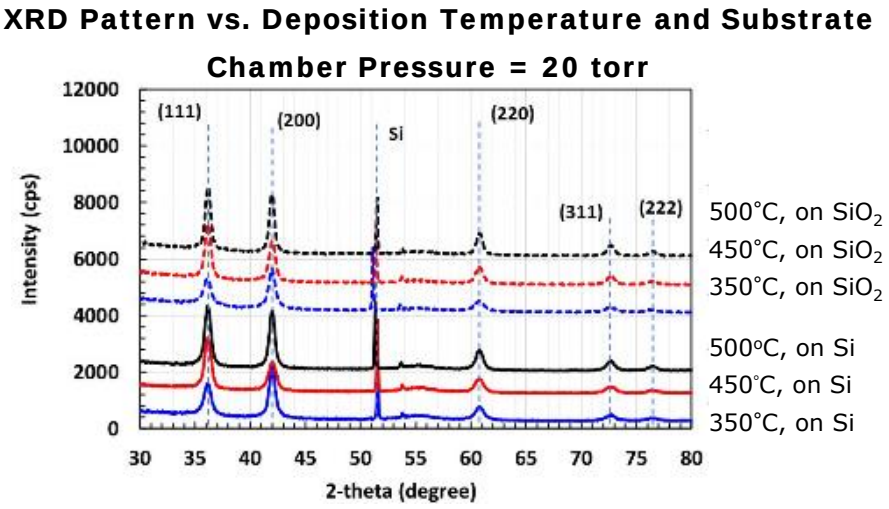
- According to SIMS analysis films deposited on Si substrate were nitrogen-rich, consistent with RBS data
- However, films deposited on SiO_2 substrate showed composition more consistent with NbN. Further investigation is needed to confirm this observation. However, RBS of the film deposited on SiO_2 at 500°C also confirmed this observation (Nb=49.0; N=50.1)

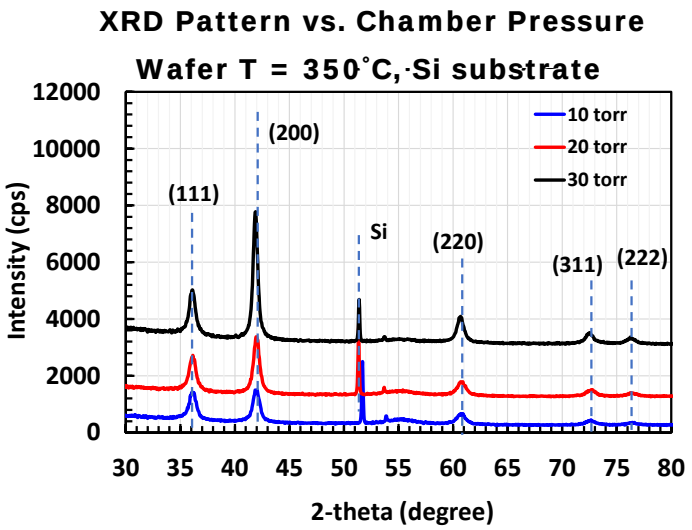




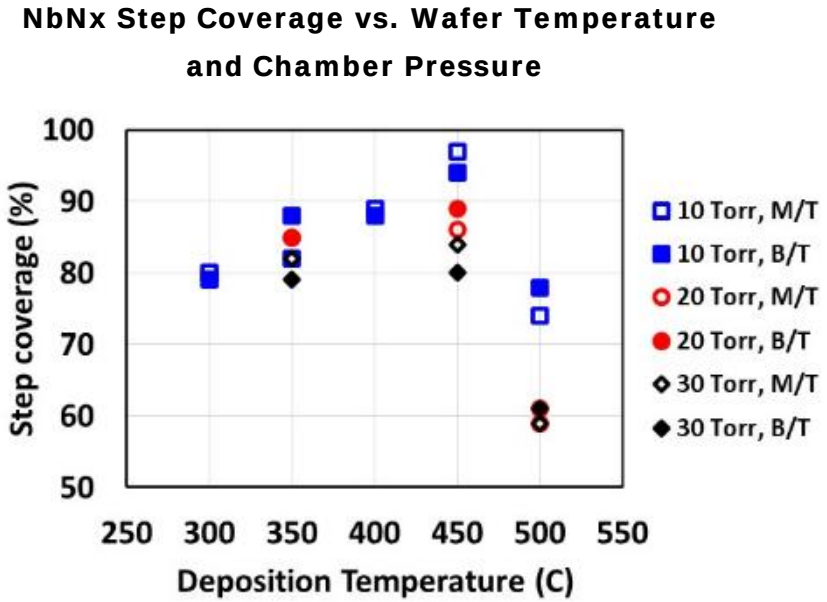
Characterization of Niobium Nitride Film
XRD and XRR Analysis

- All films deposited about 350°C were polycrystalline
- XRD results showed peaks correlated with Nb_4N_5 structure
- Relative peak intensities of 111 and 200 reflections changed with deposition temperatures but no obvious effect of chamber pressure or substrate was observed
- Film density measured by XRR was ~ 6.7 g/cm^3 at 350°C and increased to 7.3 g/cm^3 at 500°C wafer temperature



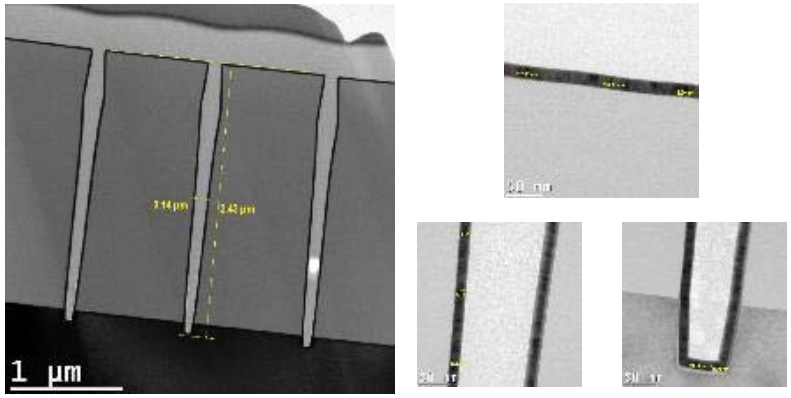


Characterization of Niobium Nitride Film
Step Coverage Optimization



3/30/5/30 x 500cy, NH_3 Thermal ALD; AR ~ 15-18
M/T = Middle Thk/Top Thk (%)
B/T = Bottom Thk/Top Thk (%)

- The effect of wafer temperature and chamber pressure on step coverage (SC) were studied
- SC improved at lower chamber pressure
- Best SC was at 450°C and 10 torr



Top THK = 18.0 nm
Middle = 17.5 nm (SC ~ 97%)
Bottom = 17.0 nm (SC ~ 93%)

Atomic Layer Deposition of Niobium Nitride Film
Summary and Conclusions

- ALD saturation characteristics, linearity of growth and ALD thermal window were investigated on various substrates such as Si, SiO_2, Al_2O_3 and TiN.
- The ALD window of NbNx film was observed from 400 to 450°C with ALD deposition rate in 0.35-0.40 Å/cycle range.
- Best step coverage was observed at 450°C wafer temperature and 10 torr chamber pressure, ~ 95 % in trench pattern with A/R > 17
- The resistivity of NbNx film decreased gradually as the deposition temperature increased. It was 1900 µohm-cm at 350°C and decreased to 700 µohm-cm at 500°C wafer temperature
- The chemical composition correlated best with Nb_4N_5 at all conditions on Si substrate. Interestingly, Nb/N ratio was ~ 1/1 on SiO_2 substrate based on RBS and SIMS analyses. This observation will have to be investigated further to explain potential effect of the substrate on stoichiometry of NbNx film.
- The Cl impurities decreased with increase in deposition temperature and were <0.6 at % at 500°C.

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