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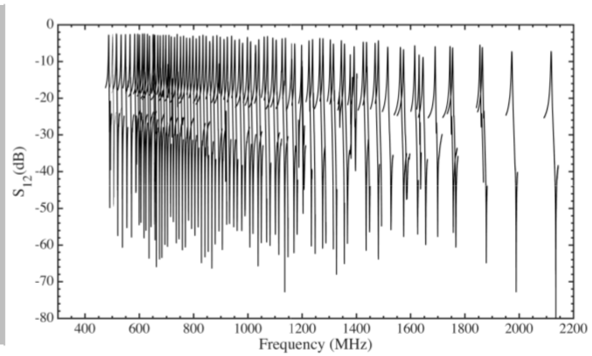

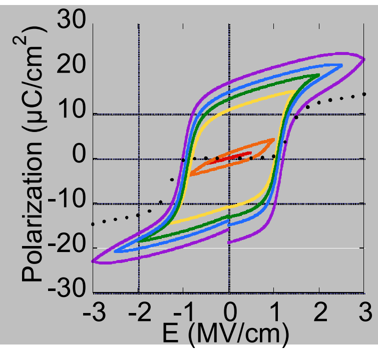

Piezoelectric RF & Ferroelectrics in Sandia MESA Fab

M.D. Henry,

PIs: Ben Griffin, Chris Nordquist, Jon Ihlefeld, Paul Davids

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Piezoelectric and Ferroelectric for Advancing Technologies at Sandia MESA Fabrication Facility

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two device technologies to couple to microelectronics

- ScAlN Development – RF filters
  - Contour Mode Resonators for RF Filters – the multifrequency promise
  - 12.5% ScAlN reactive sputtering development
  - Fabrication of CMRs - challenges

- HfZrOx Development – FTJ and NC FETS
  - HZO for tunnel junctions
  - ALD of Hf and Zr to find the right ferroelectric
  - Band Diagrams of top metal and why it matters
  - Where else would HZO work

Contour Mode Resonators

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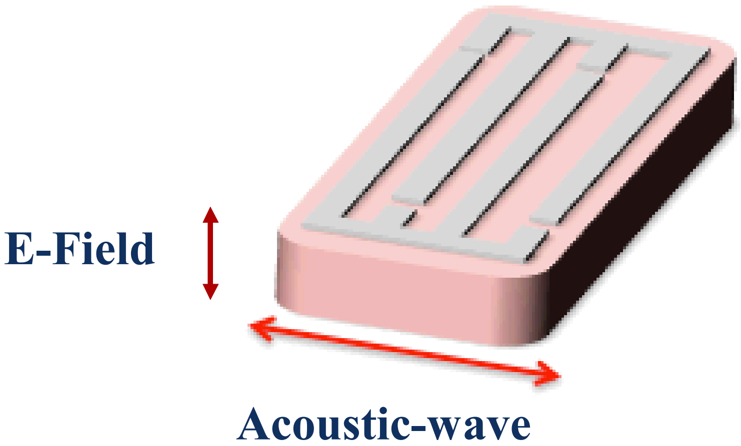
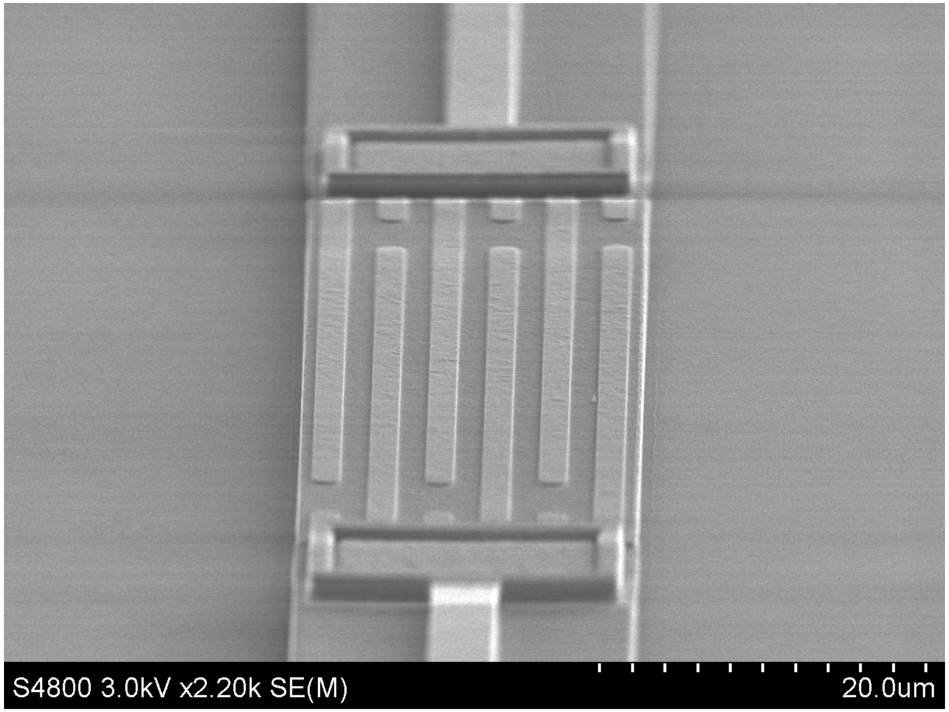




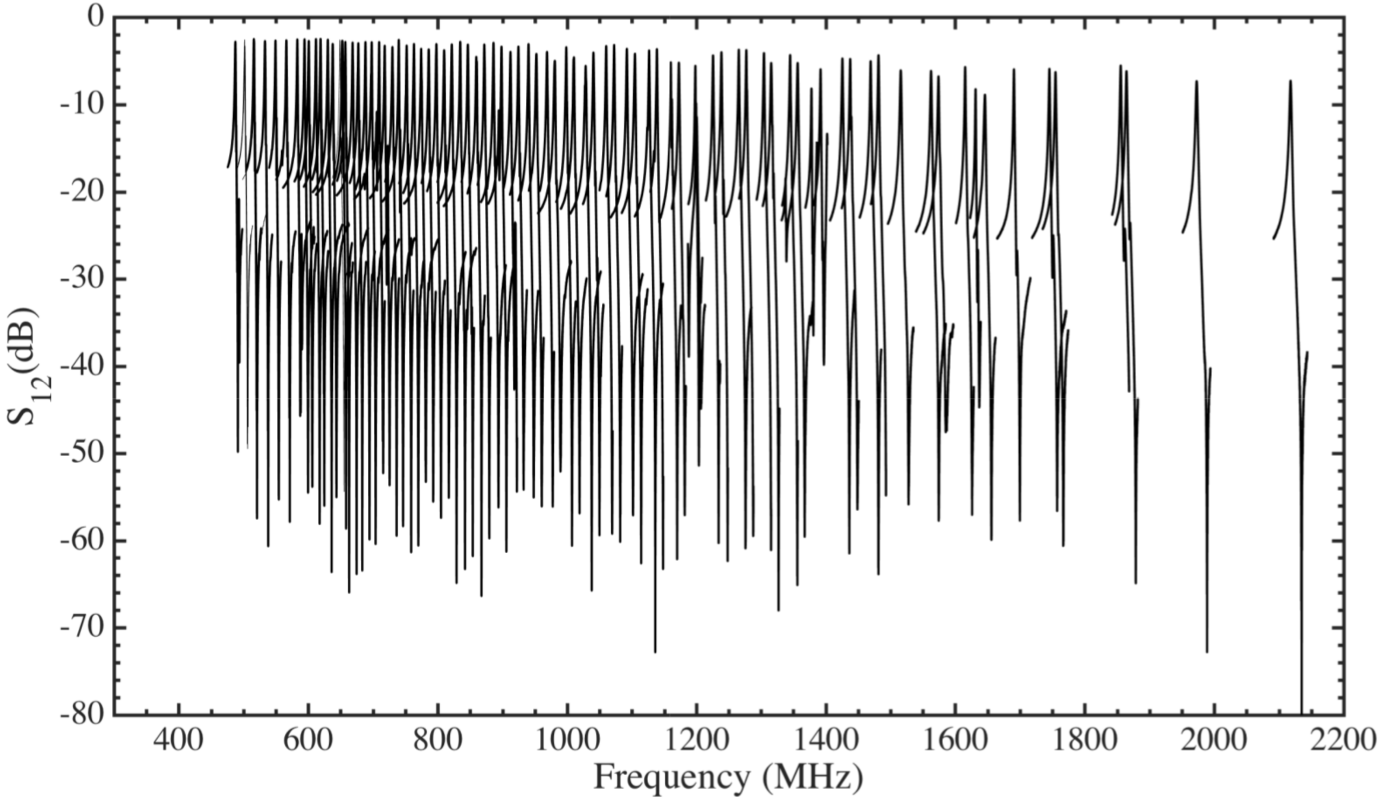
$$E\frac{\partial^2 u}{\partial x^2} = \rho \frac{\partial^2 u}{\partial t^2}$$

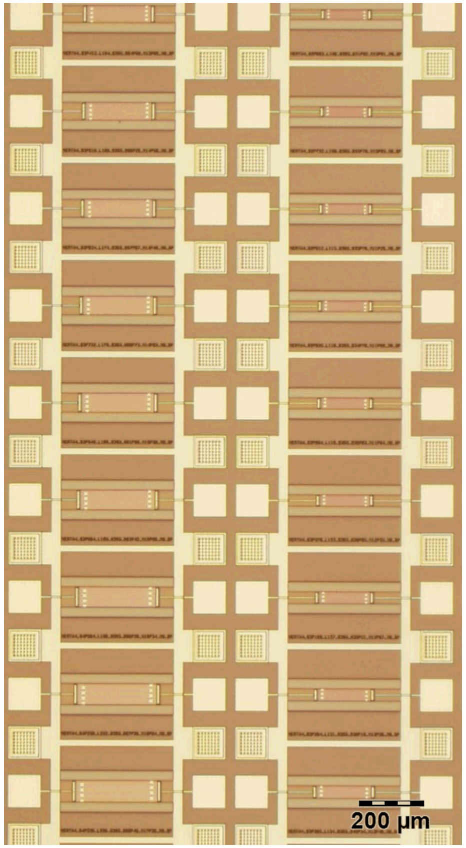
$$f = \frac{v}{\lambda} = \frac{1}{2w} * \sqrt{\frac{\sum E * t}{\sum \rho * t}} \qquad w = \frac{n\lambda}{2}$$

Contour mode resonators take an electric field (z axis) and create an acoustic wave (x axis) using the piezoelectric properties (d_{31}) of a film (AlN). This permits lithography to define many frequencies on the same piezoelectric film.

M. D. Henry, J. Nguyen, T. R. Young, T. Bauer, and R. Olsson, "Frequency Trimming of Aluminum Nitride Microresonators Using Rapid Thermal Annealing," *JMEMS,* pp. 1-1, 2013.

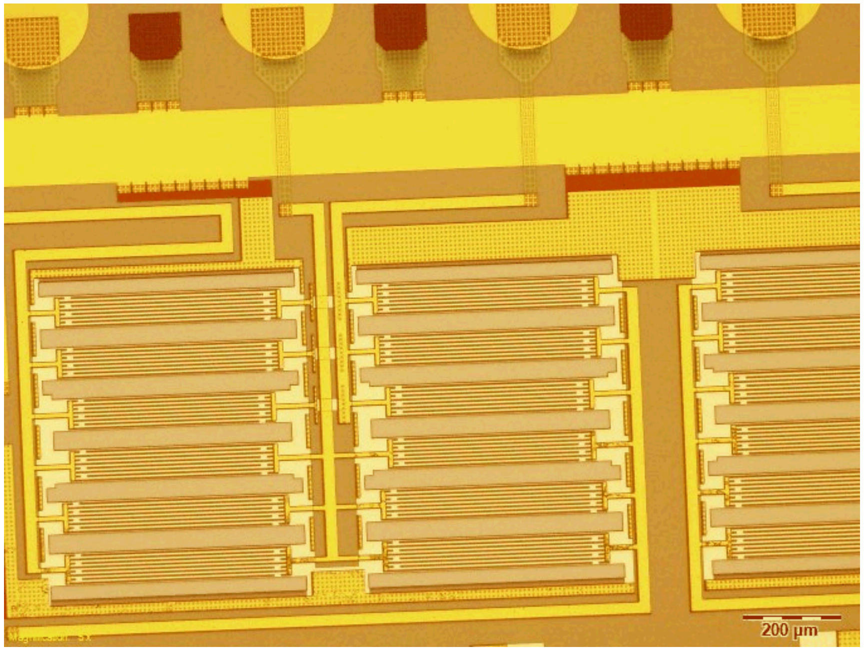
Many Contour Mode Resonators

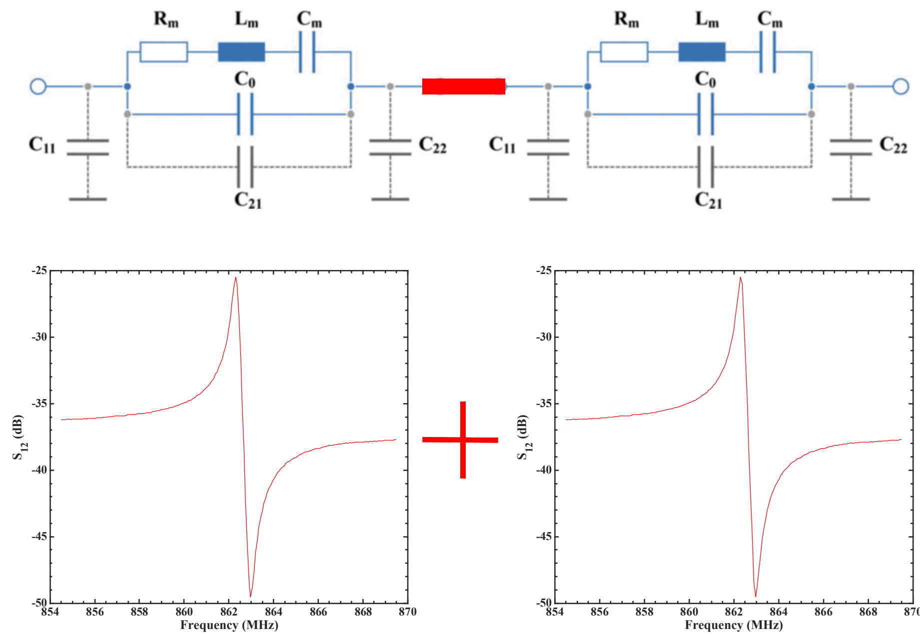




With CMR, a wide range of resonances can be achieved on the same wafer, and on the same die. Above is a die of resonators created in 750 nm thick AlN.

Resonators to RF Filters

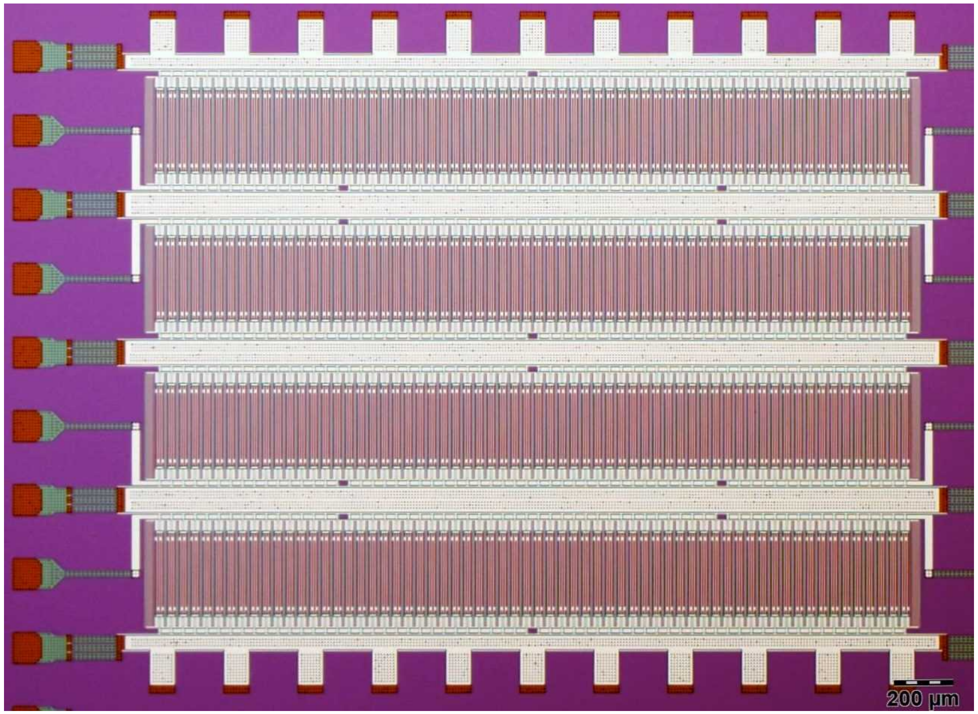


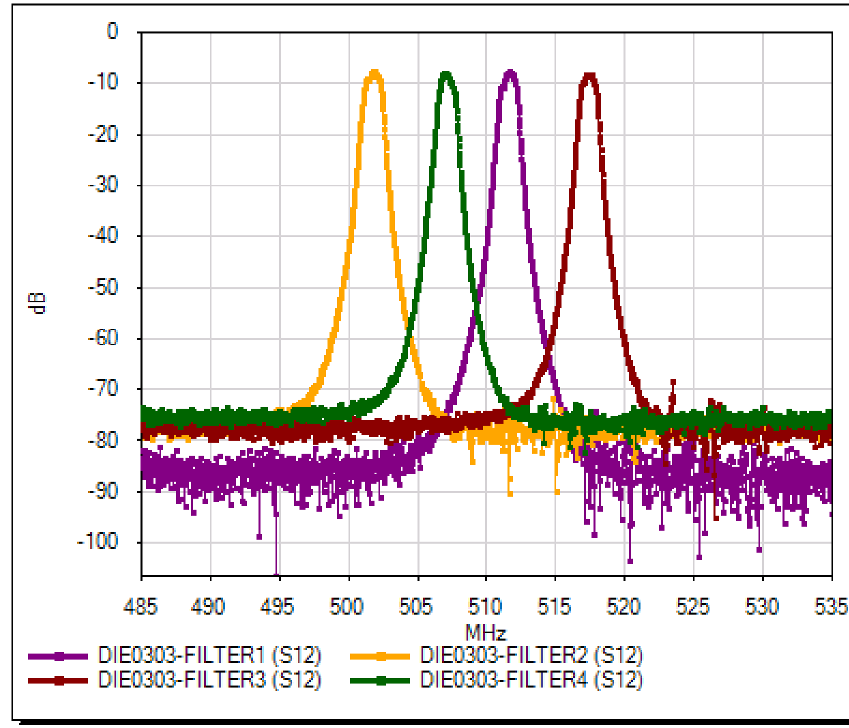


The value proposition for contour mode resonators is that when configured in banks, RF filters can be created. Limitations for this technology is based on bandwidth, band rejection, and insertion loss which are dependent upon the piezoelectric kt^2 and resonator Q factor.

Resonators to RF Filters

Small changes in the lithographic layout of the CMRs, can control the bandpass frequency. This means that multiple filters of different frequencies can be on the same piezoelectric film.



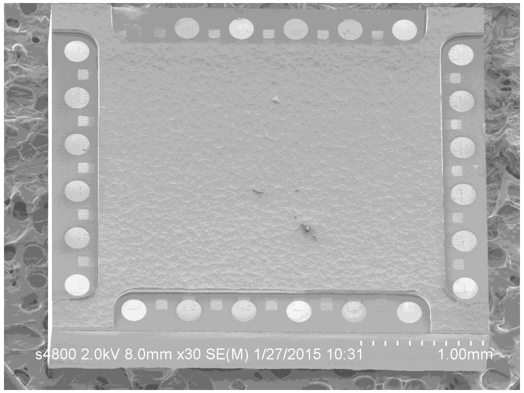


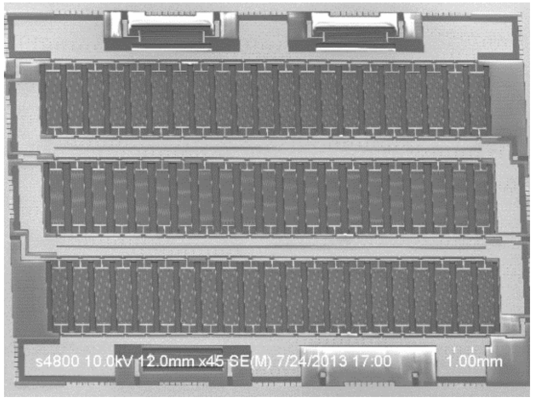
This enables 4 times the devices utilizing only one film for 10MHz to 10 GHz RF filters using the same film (aka significantly cheaper).

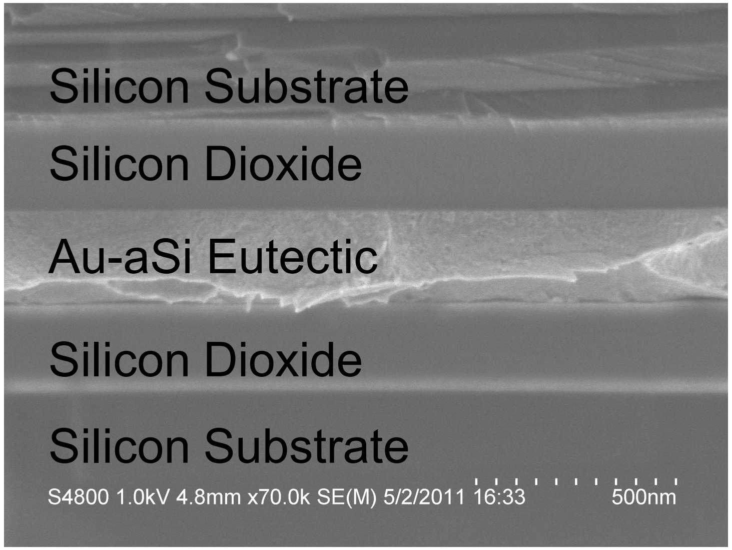
M. D. Henry et al, "Wafer-level packaging of aluminum nitride RF MEMS filters, ECTC , 2015 IEEE 65th, San Diego, CA, 2015.

Hermetic Wafer Level Packaging Resonators and RF Filters

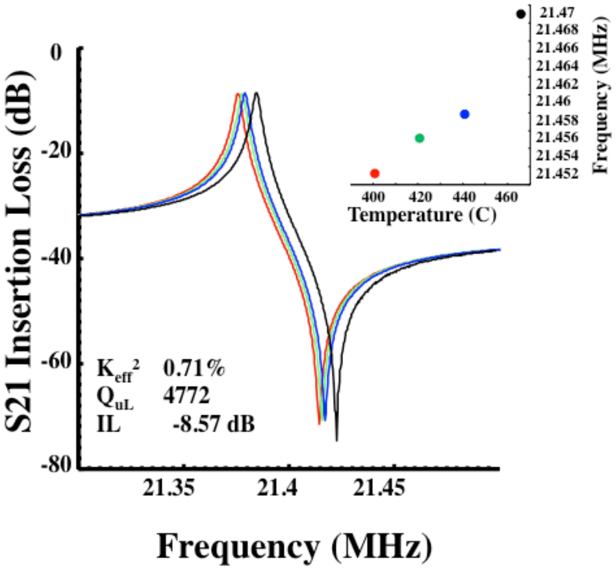
The issue of dicing the suspended filters is quickly solved by wafer level packaging – bond the etched lid wafer to the resonator wafer and plasma thin until the pads are revealed.

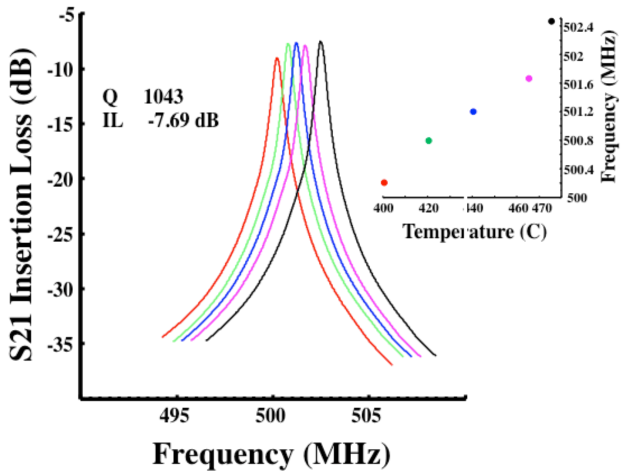


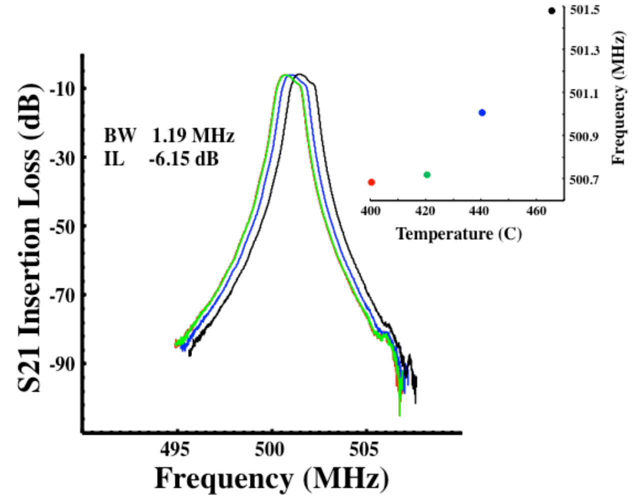


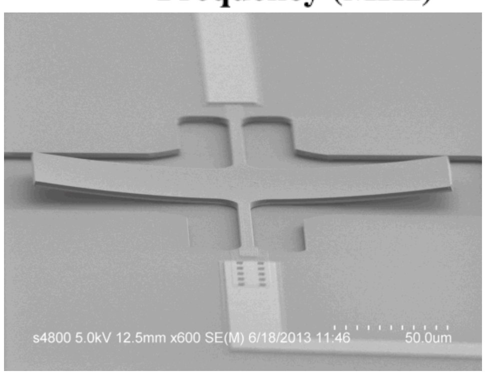


Frequency Trimming with the RTA

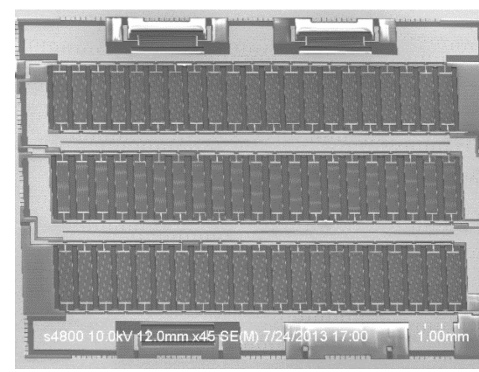








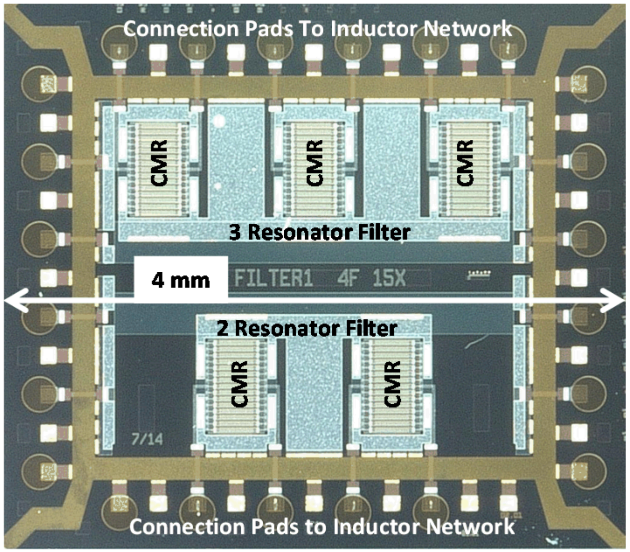
$$f=\frac{\nu}{\lambda}=\frac{1}{2w}*\sqrt{\frac{\sum E*t}{\sum \rho *t}}$$

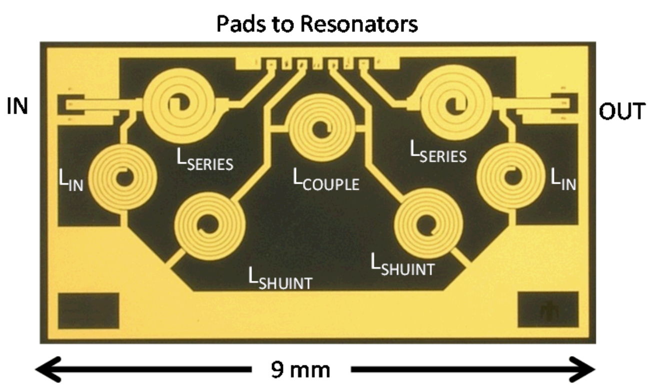


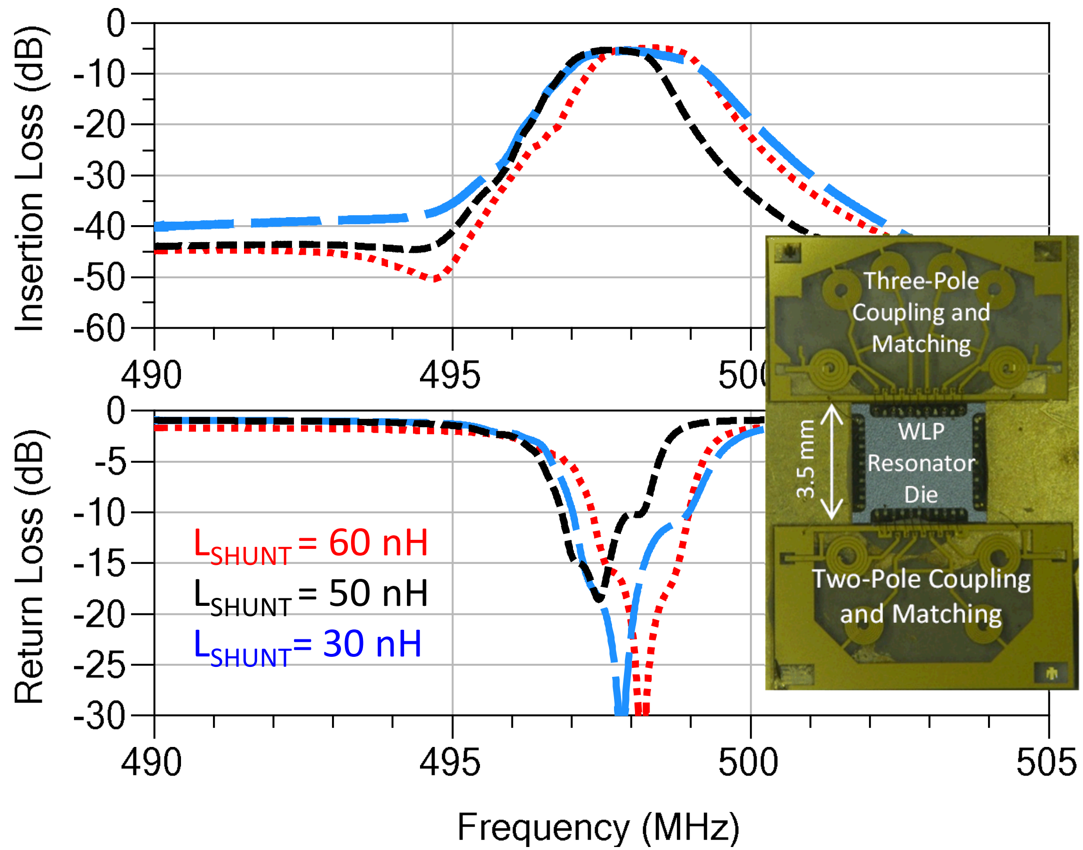
Using stress control over the metal layers, RTA can relax film stress to increase acoustic velocity. Chips can now be individually trimmed to desired frequency increasing the wafer yield.

M. D. Henry et al, "Frequency trimming of AlN microresonators using RTA" JMEMS, 2013.

Bandwidth Extension with Inductors







Using an inductor ‘pi’ coupling, output capacitance can be resonated with an on-chip surface spiral inductor and then inductively coupled to another filter bank with the input capacitance inductively resonated out.

Nordquist, C.D. et al, “Inductive Coupling for Increased Bandwidth of Aluminum Nitride Contour-Mode Microresonator Filters”, IEEE International Microwave Symposium 2016.

Another Route for BW increase - Sc

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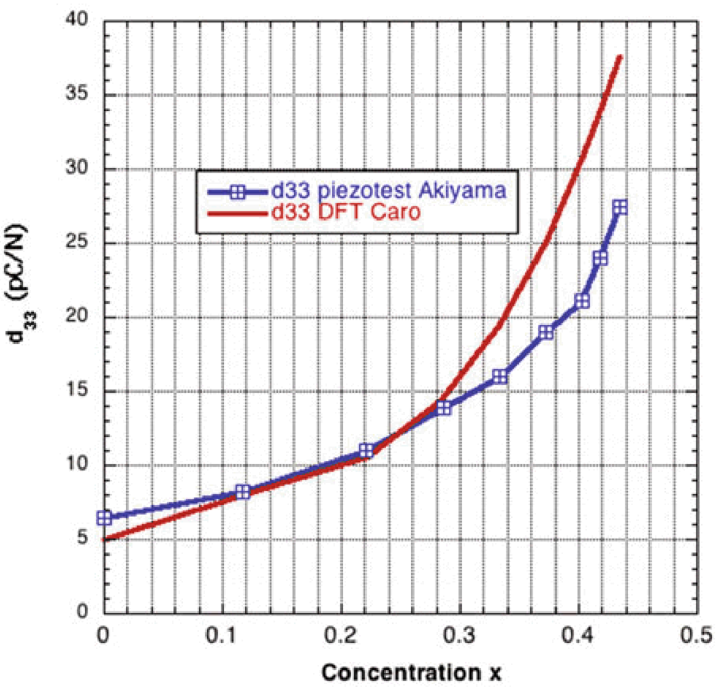
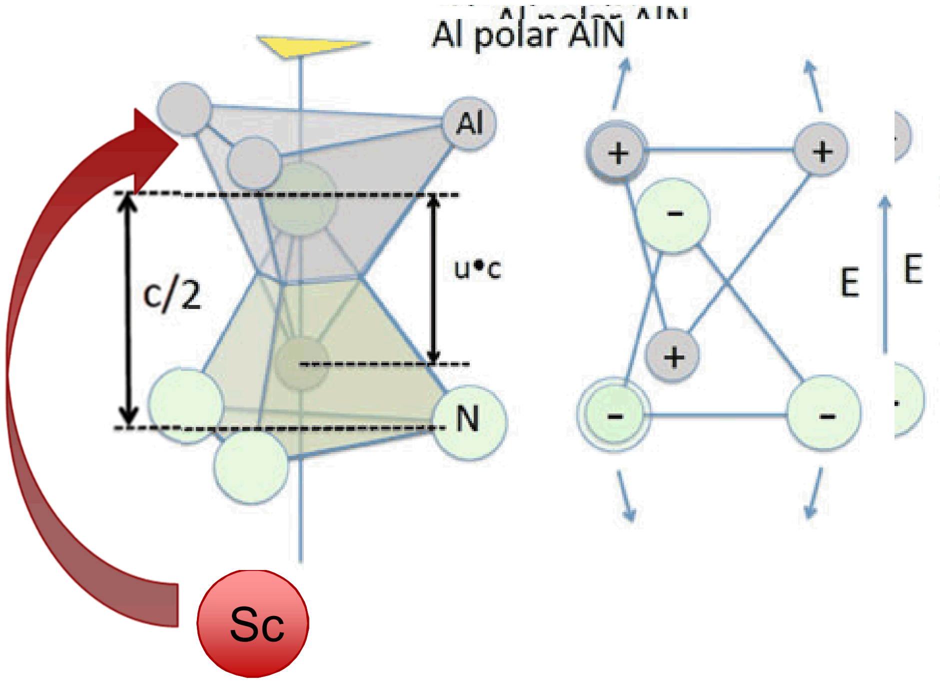
The route to better devices shows promise in increases in the d_{31} from Sc incorporation in the AlN matrix. This would give better kt^2 if Q factor is maintained.





$$k_{eff}^2 = \frac{f_p^2 - f_s^2}{f_p^2} \sim \frac{d_{31}^2 E}{\epsilon}$$

Substitutional replacement of Al with Sc, is expected to increase the ionic displacements in electric fields.

P. Muralt, in *Piezoelectric MEMS Resonators* (Springer, 2017), pp. 3-37.

Inclusions in Reactively Sputtered 12.5% ScAlN Films on Si (100)

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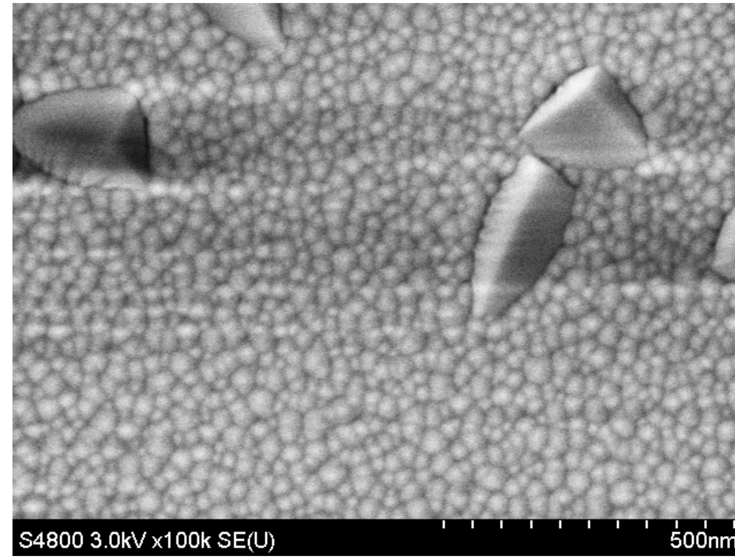
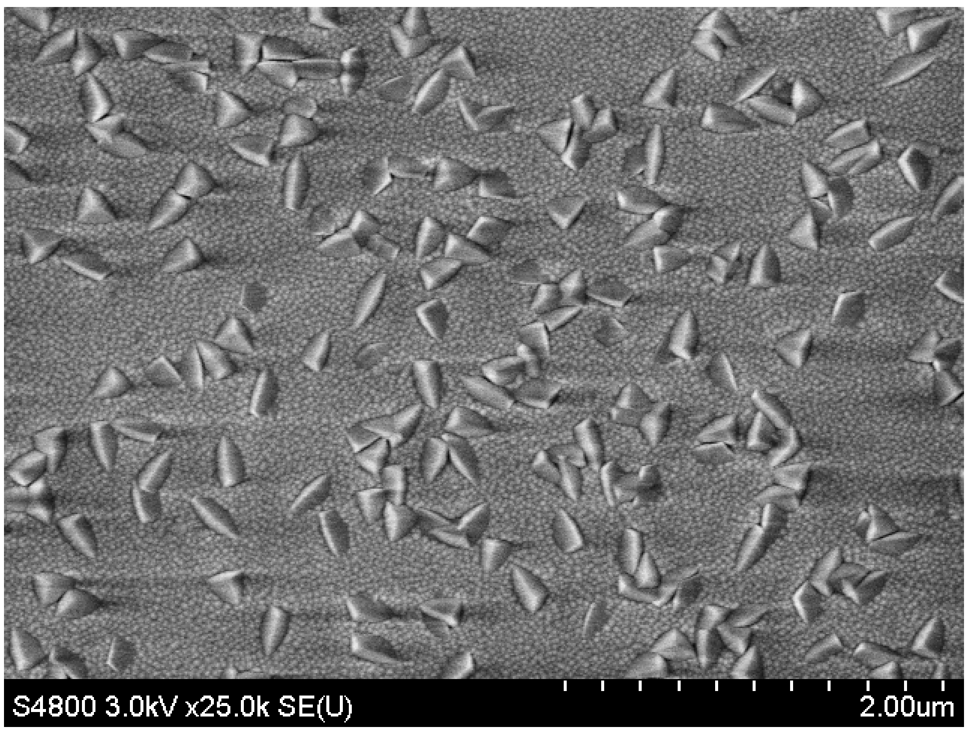
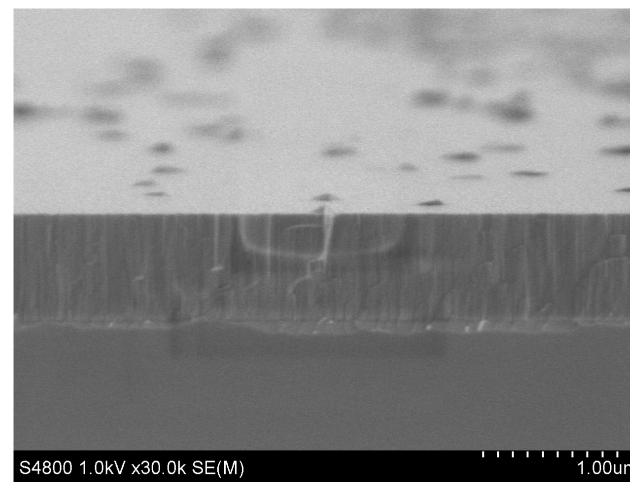
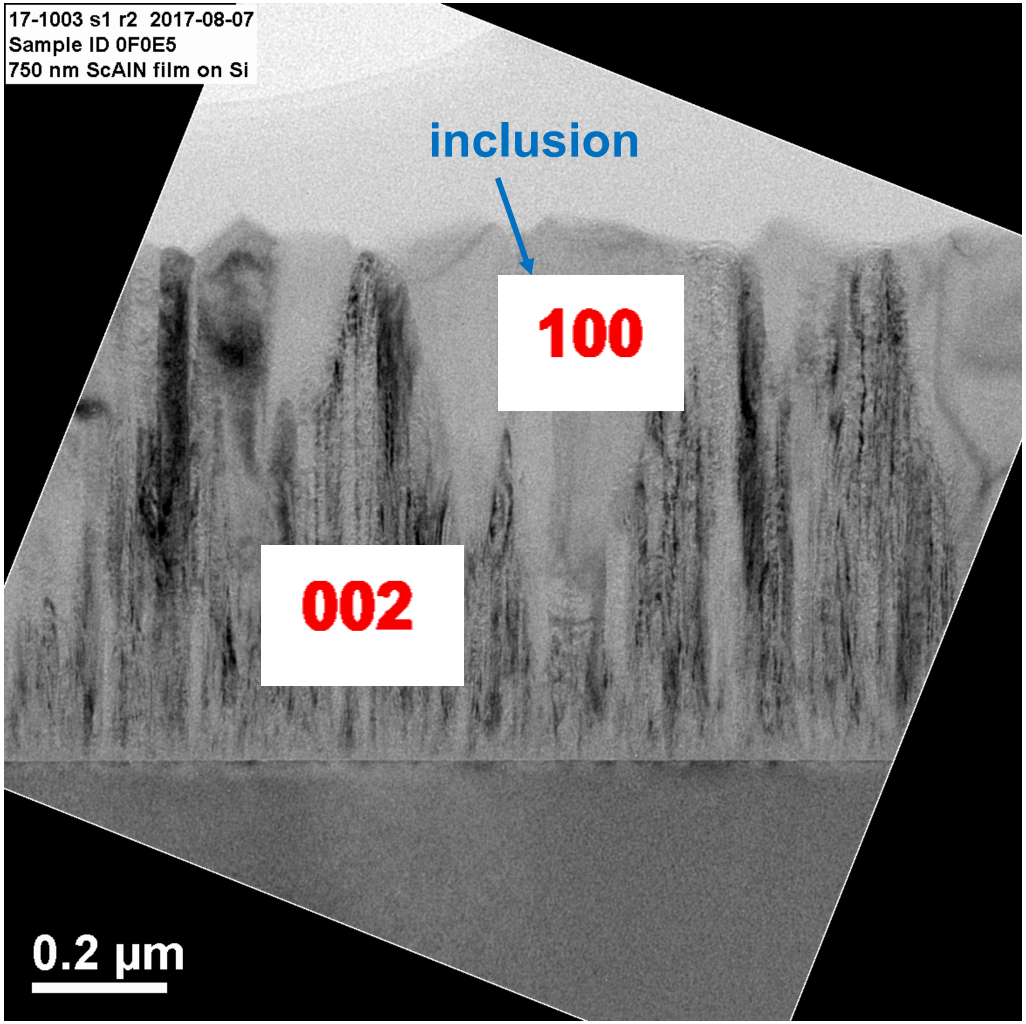
Scientific literature shows the predicted increase in d_{31} but strange inclusions/hillocks arise in the film as Sc content increases.

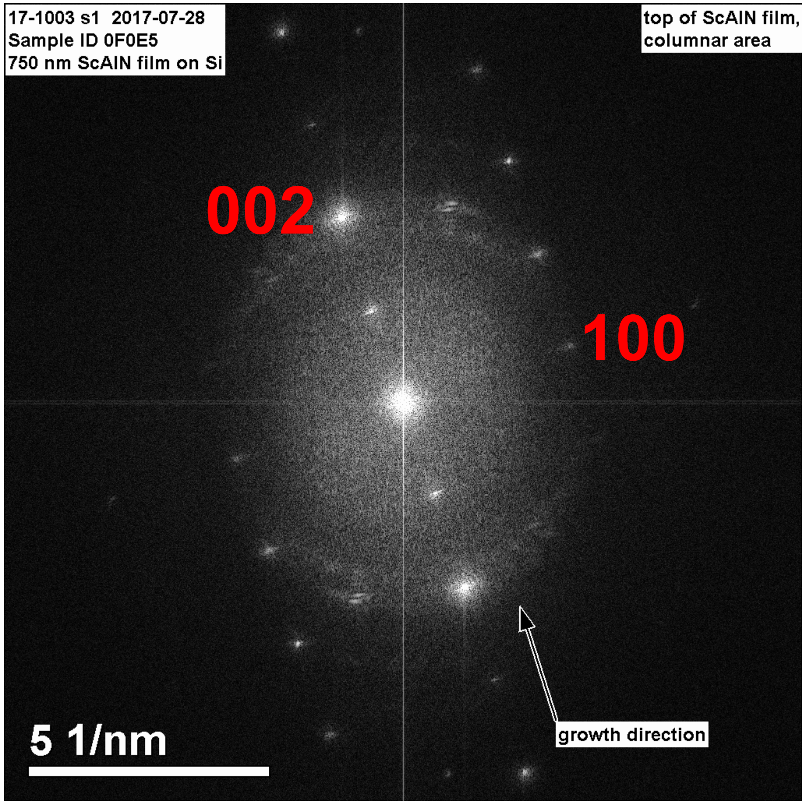




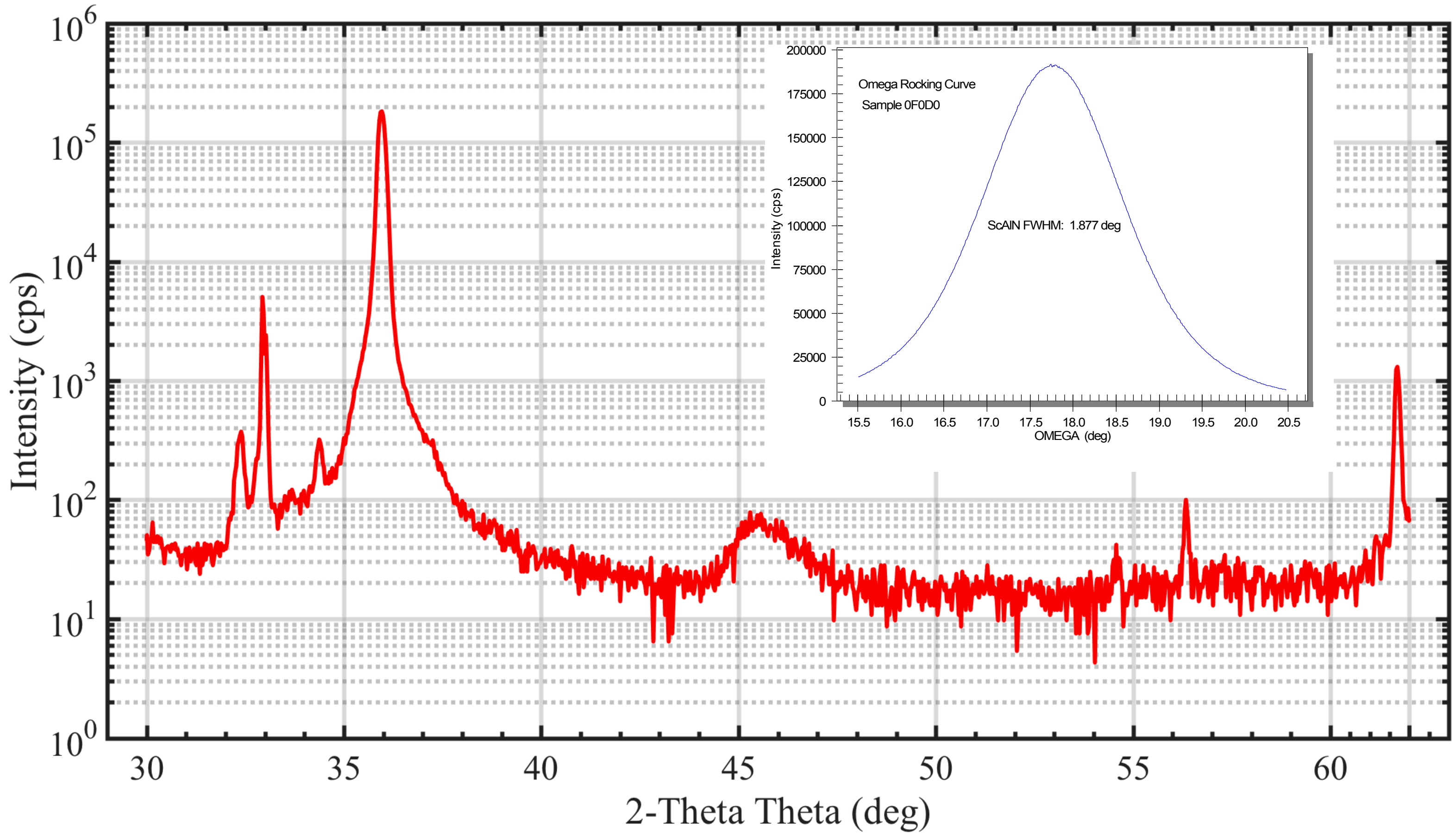


TEM of 12.5% ScAlN on Si and Inclusions – a (100) growth



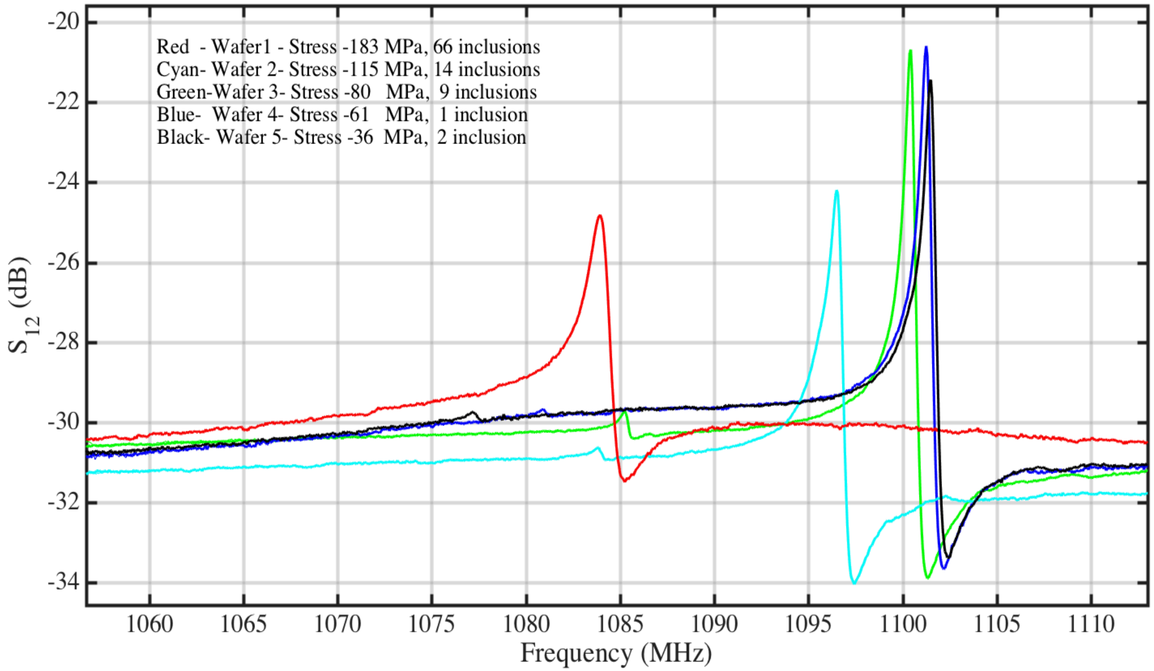


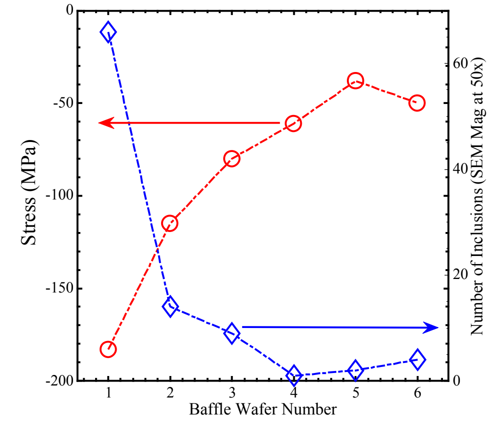
Rocking Curve and XRD ScAlN on Si (100)

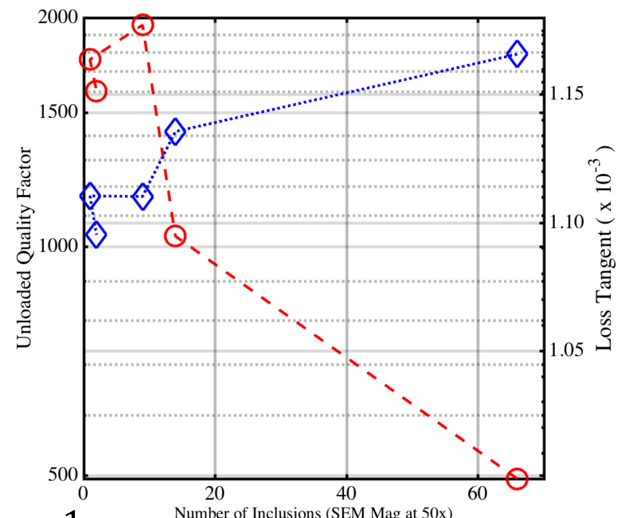


Two very clear peaks… (100) at ~33 deg and (002) at ~ 36 deg.
So with the inclusions looking to be the (100) growth, and rocking curves still suggesting highly oriented films… what is the result for CMRs?

Top Electrode Resonators Inclusions Impact on Q-factor





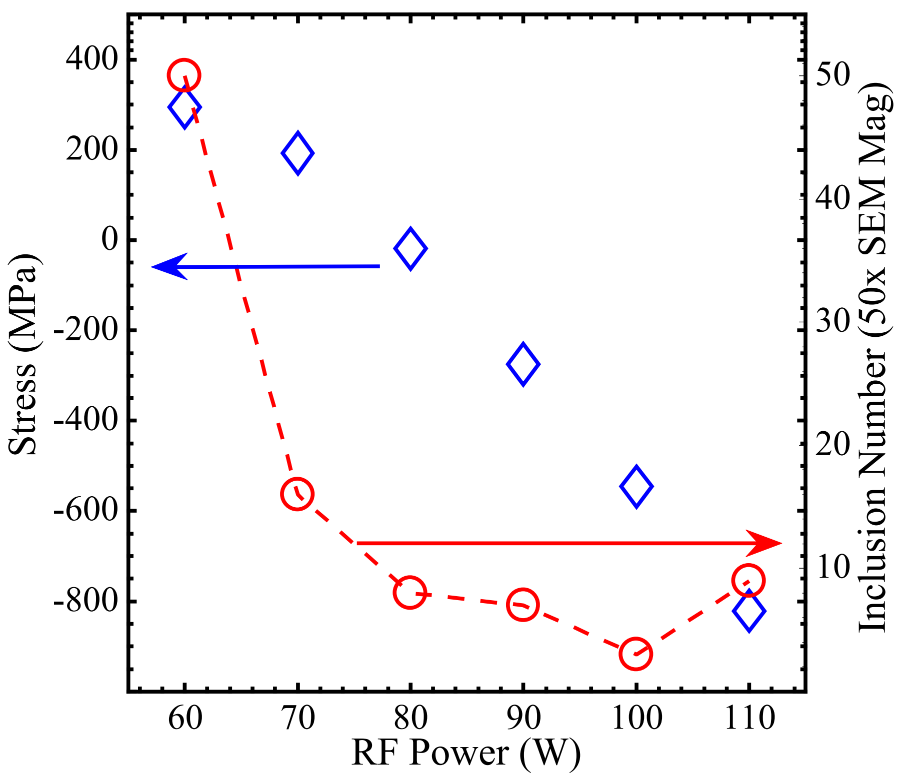


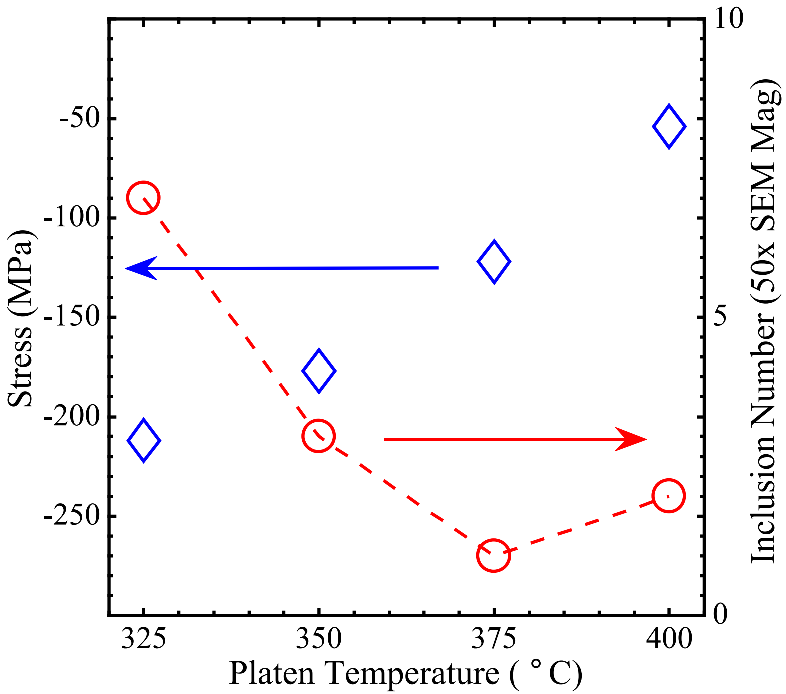
With fabrication, it is reasonable to assume all wafers are processes the same. This suggests other loss factors are responsible for the differences between the wafers. This should rule out other typical Q loss mechanisms including anchor, electrical-resistive, air dampening, and surface losses. This leaves acoustic scattering off 100 as the likely culprit.

$$Q_{UL} = \left(\sum_i \frac{1}{Q_i}\right)^{-1}$$

Dialing in Stress During Reactive Deposition - RF Power and Temperature

FOM relies on both Q and kt^2, so the value of increased Sc becomes negated if the 100 growth is not controlled.
RF power is the significant knob for controlling stress and inclusion suppression.

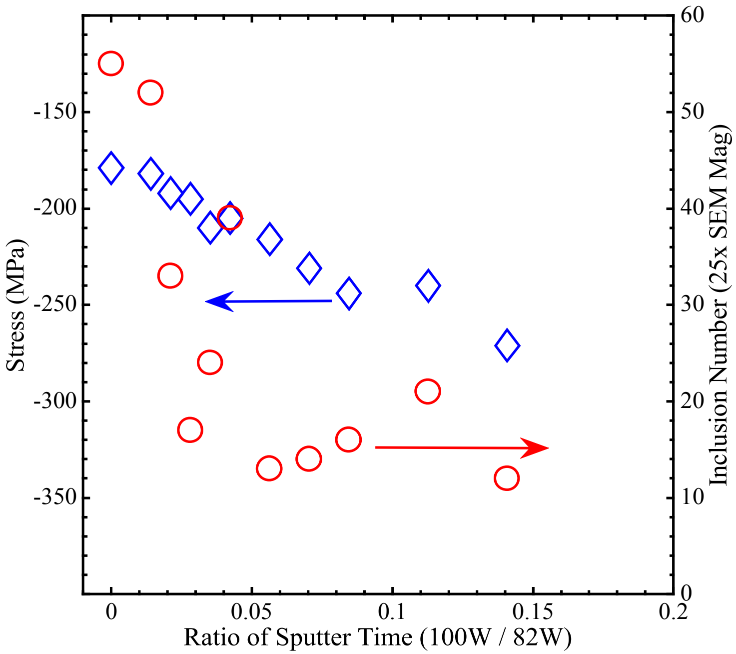


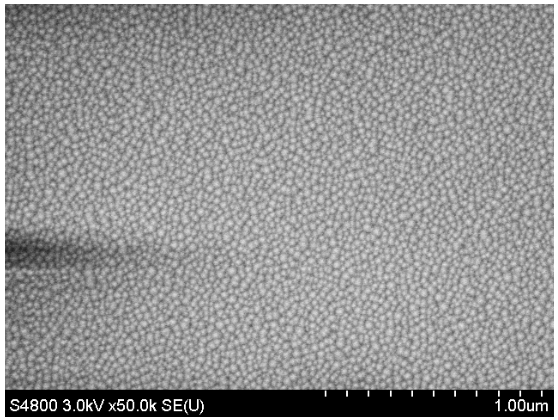


Two Step 12.5% ScAlN on Si (100) Deposition Control

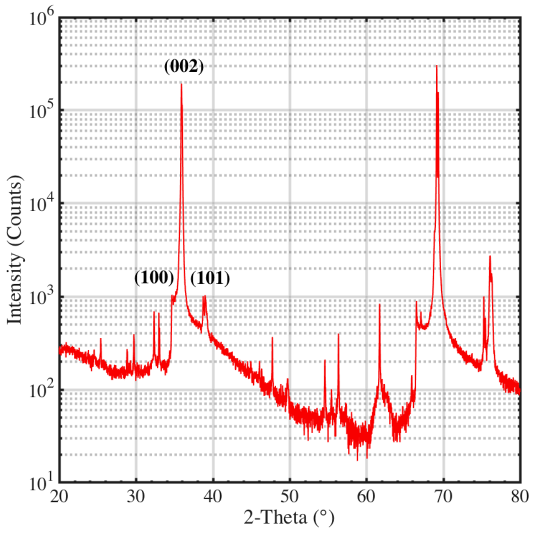
Higher RF (100 W) creates a high stress but this is counter productive to released devices where Euler buckling can occur. The solution is to start with higher compressive stress then move the film back to low stress.

Film thickness average of 751.4 nm (std dev of 5.2 nm).

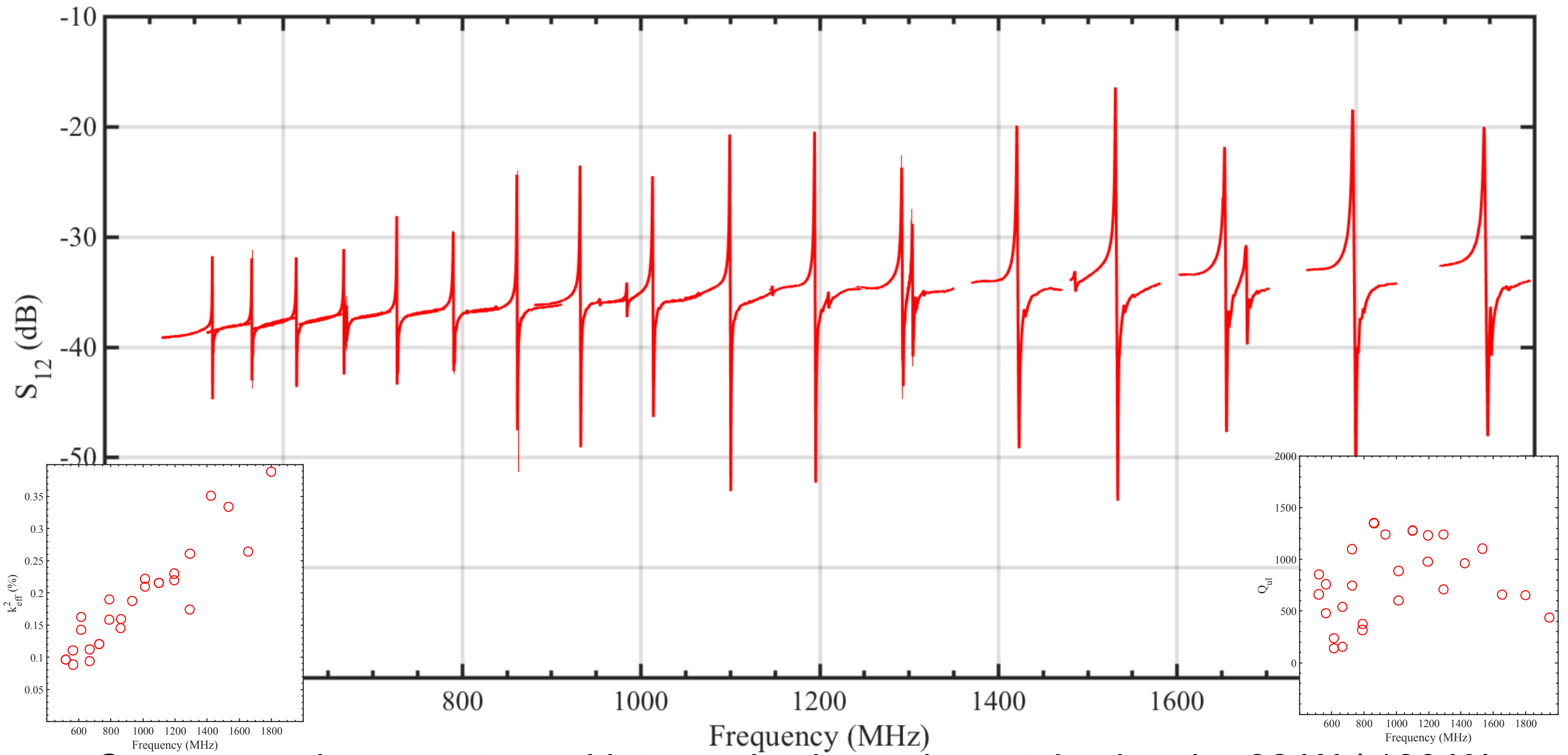




Rocking curve at 1.884 deg.



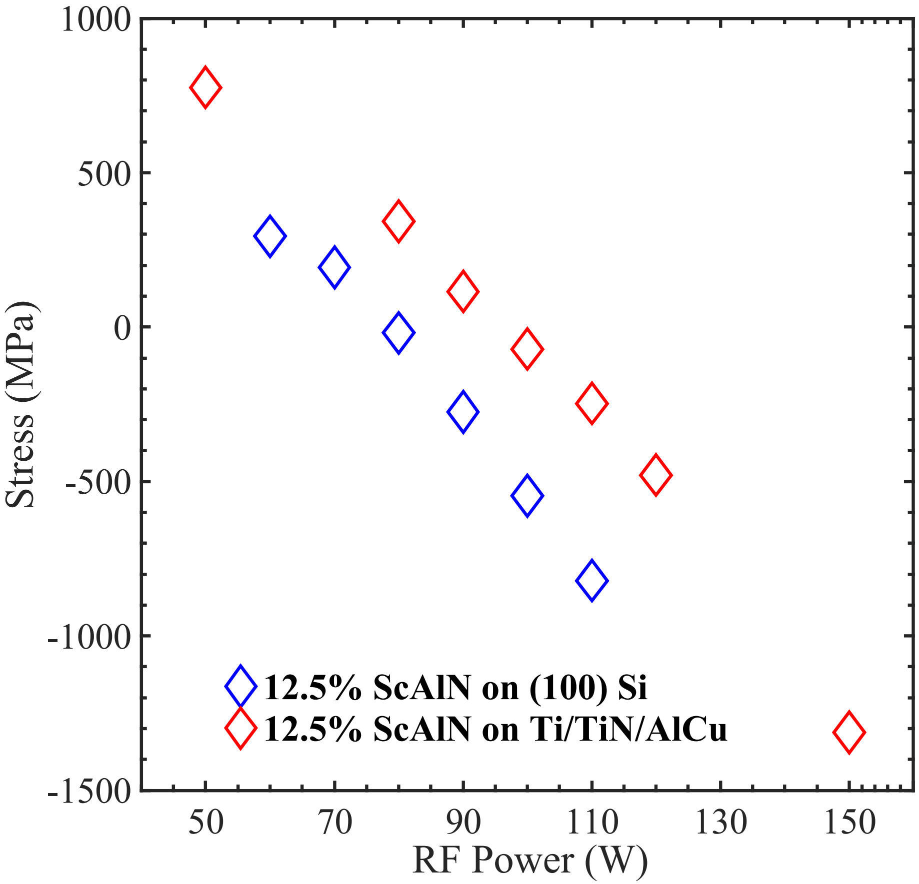
Suppression of Inclusions for ScAlN CMRs on Si (100)

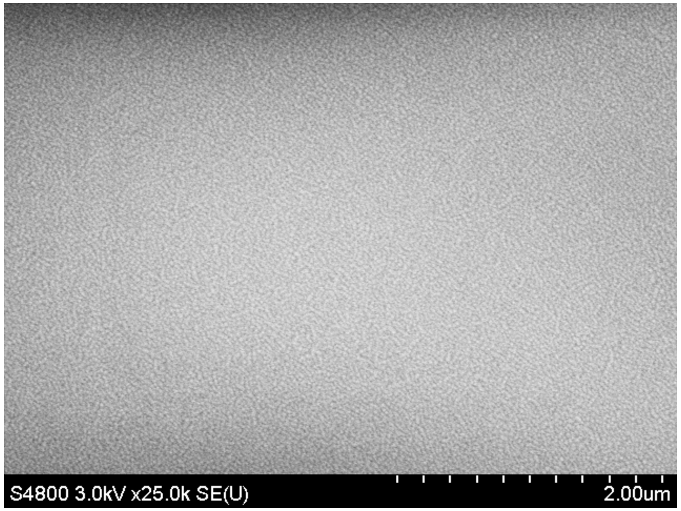


Contour mode resonators with top only electrode metal using the 82 W / 100 W RF deposition show good RF S_{12} performance. The 756 nm $Sc_{0.125}Al_{0.875}N$ film was under -182 MPa stress and rocking curve of 1.88 degrees.

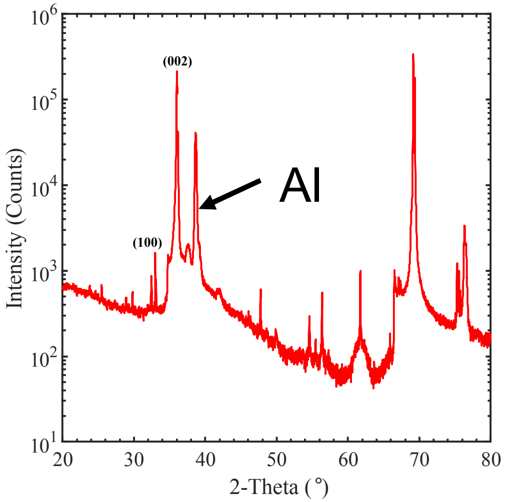
Dialing in Stress During Deposition on Ti/TiN/AlCu

What about having a top/bottom electrode?
What metal do I orient with (CMOS compatable?)

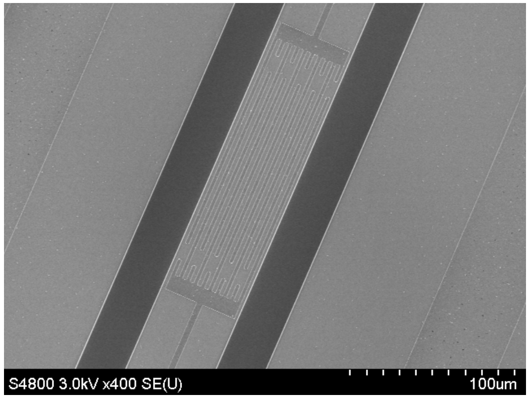




Two step deposition (100 W 40 seconds with 75 W 660 seconds). 1.524 deg rocking curve.

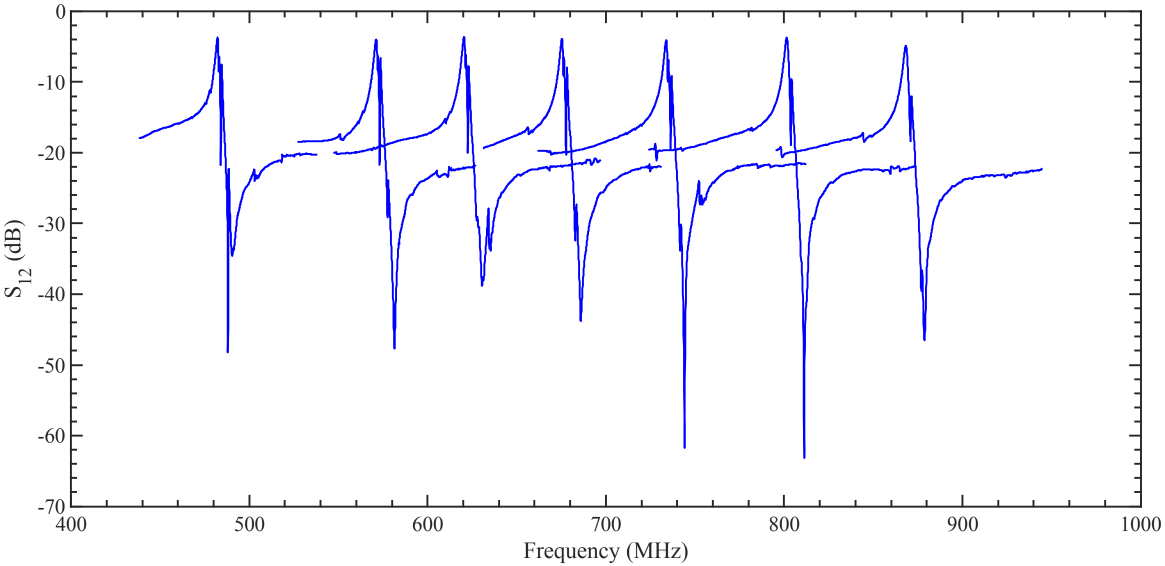


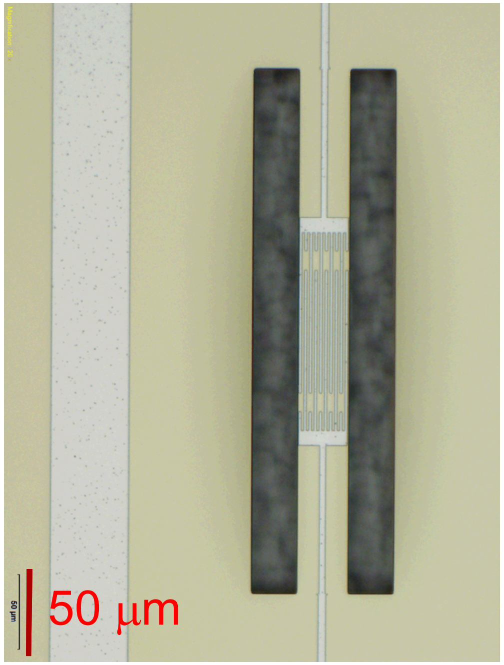
12.5% ScAlN CMRs on Ti/TiN/AlCu



Kt^2 values are seen in the 2.4% range suggesting the expected increase in electrical mechanical coupling was achieved. Strong parallel peak resonances suggest good Q factors as well.

It seems that we have a method to migrate to 20% Materion targets.

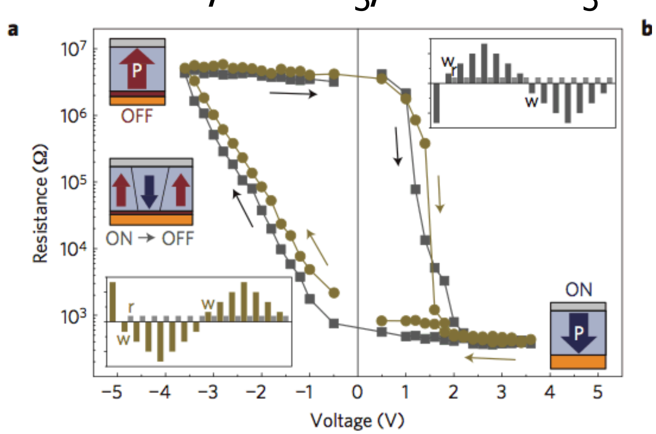


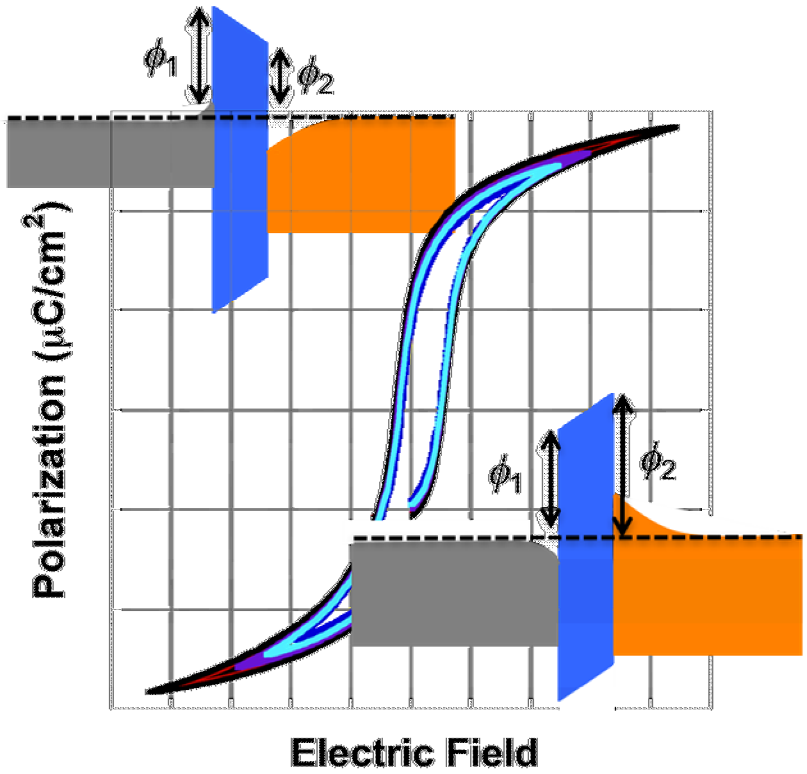


Novel Solution to the need for dense CMOS, memory: Ferroelectric Tunnel Junction (FTJ)

- An equilibrium approach will enable for reliable and repeatable device operation
- Ferroelectricity is an equilibrium phenomena of switchable polarization that can be used to prepare tunnel junctions
- A switchable, permanent polarization enables switchable, permanent resistances
  - Must be thin enough for tunneling (<5nm)

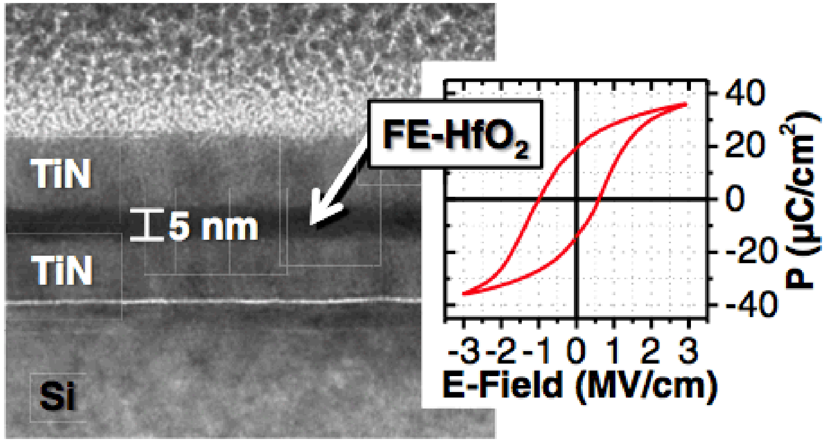
$Pt/BaTiO_3/Nb:SrTiO_3$





Approach so far: Ferroelectric HfO_2

- ALD-deposited, doped, HfO_2 has recently been discovered to possess ferroelectric signatures
- Stable ferroelectric response to at least 3 nm thicknesses*
  - "Leakage current limits scaling below 5 nm" (for FRAM)♯
- ALD HfO_2 is scalable, Fab-compatible, and inexpensive
- We will:
  1. Prepare ALD doped-HfO_2
  2. Prepare FTJs with differing electrodes
  3. Integrate FTJs into prototype memristor designs



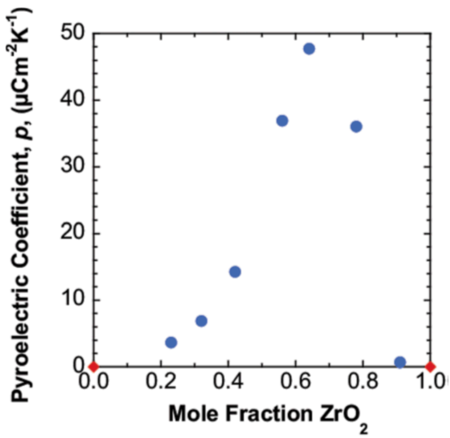
Risks: New research area on new material – many unknowns

*Materlik, et al., J. Appl. Phys. 117, 134109 (2015)

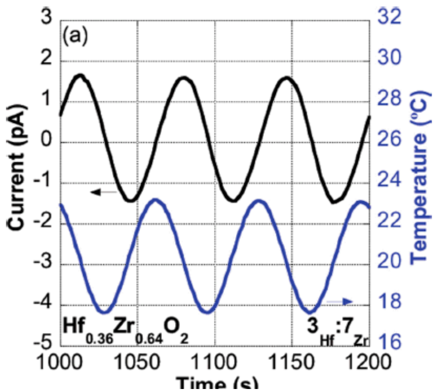
♯Müller, et al., ECS J. Solid State Sci. Tech. 4(5) N30-N35 (2015)

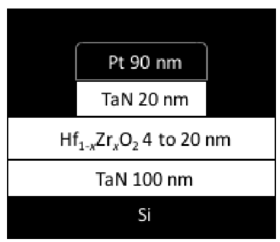
Park, et al., Adv. Mater., 27, 1811, (2015)

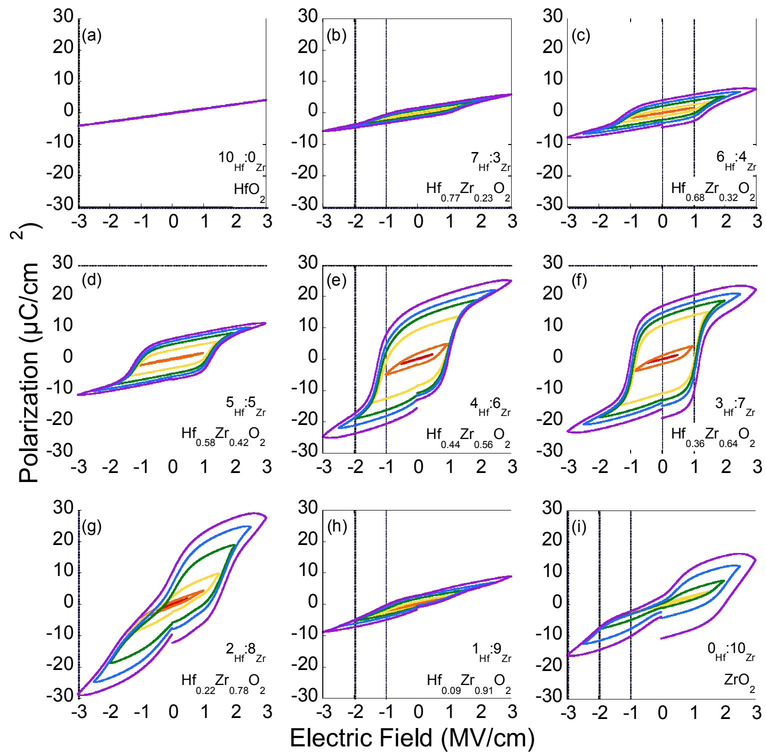
Sandia's Solution: HfZrOx

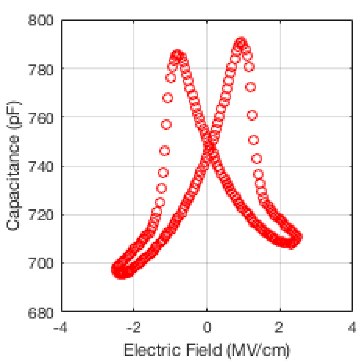


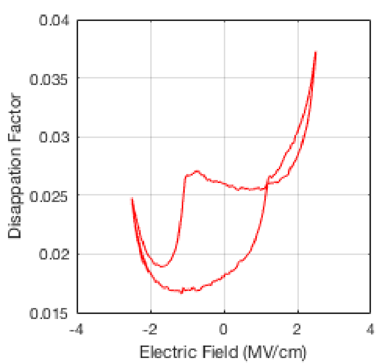
At 20 nm thick, a good ferro/pyroelectric response was found with a Hf and Zr ALD mixture. Optimal Zr content of ~ 65% is consistent with other's findings.











Smith,S. et al., APL, **110**, 072109 (2017).

What metal stack and thickness is needed to Obtain FTJ with HZO?

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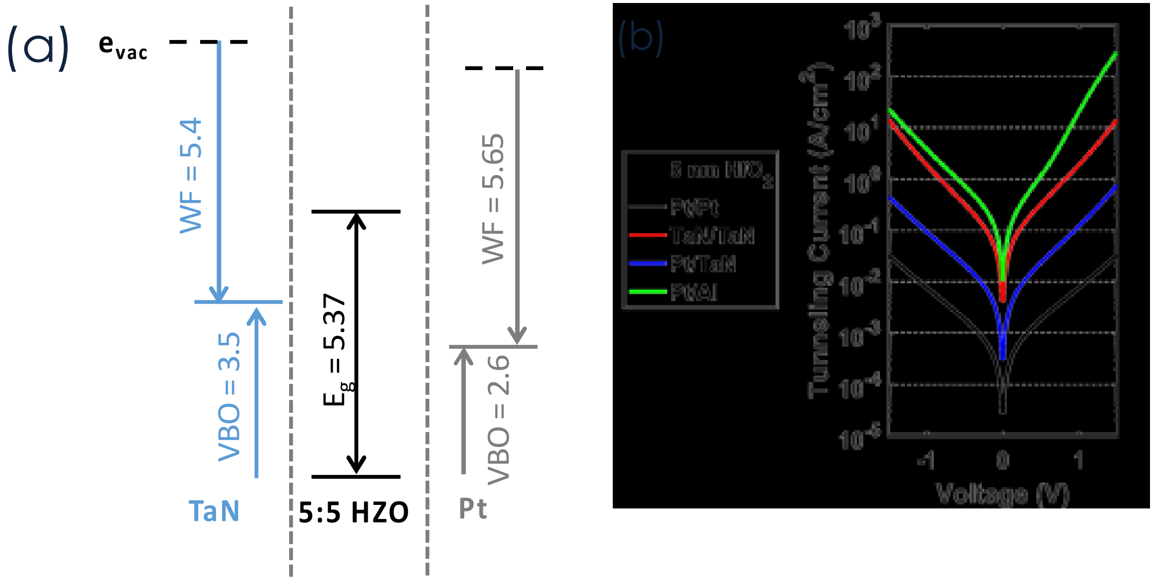
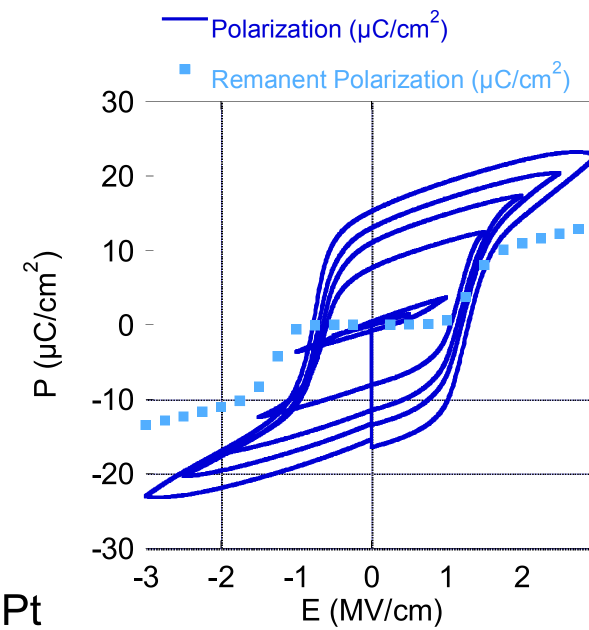




An example of the band offset measurements, here for TaN and Pt with (Hf,Zr)O_2 made for various potential electrodes, with modeled tunneling currents, based off of band offset measurements for 5 nm of (Hf,Zr)O_2.

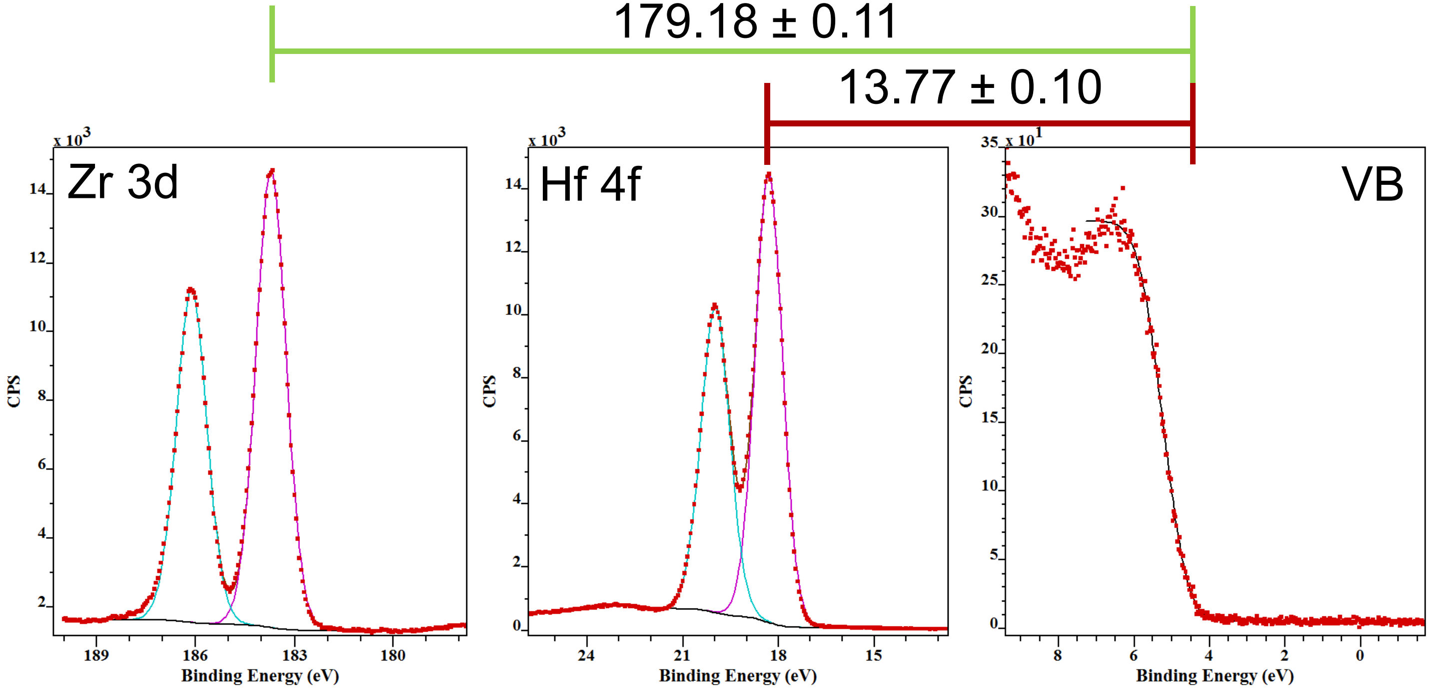
$Hf_{0.36}Zr_{0.64}O_2$ with TaN bottom and Pt top electrodes annealed to 600 °C for 30 s in N_2

For an ideal FTJ, asymmetry would be best (high resistance in one state with a lower resistance in the other). Two things needed now, HZO polarization at 5 nm and VBO and WF to get asymmetry – punchline… not there yet.

Brumbach, M. et al., presented at AVS - Tampa (2017).

XPS for VBO
Effect of different core levels

For 7 different samples of HZO measured over the course of ~24 months…



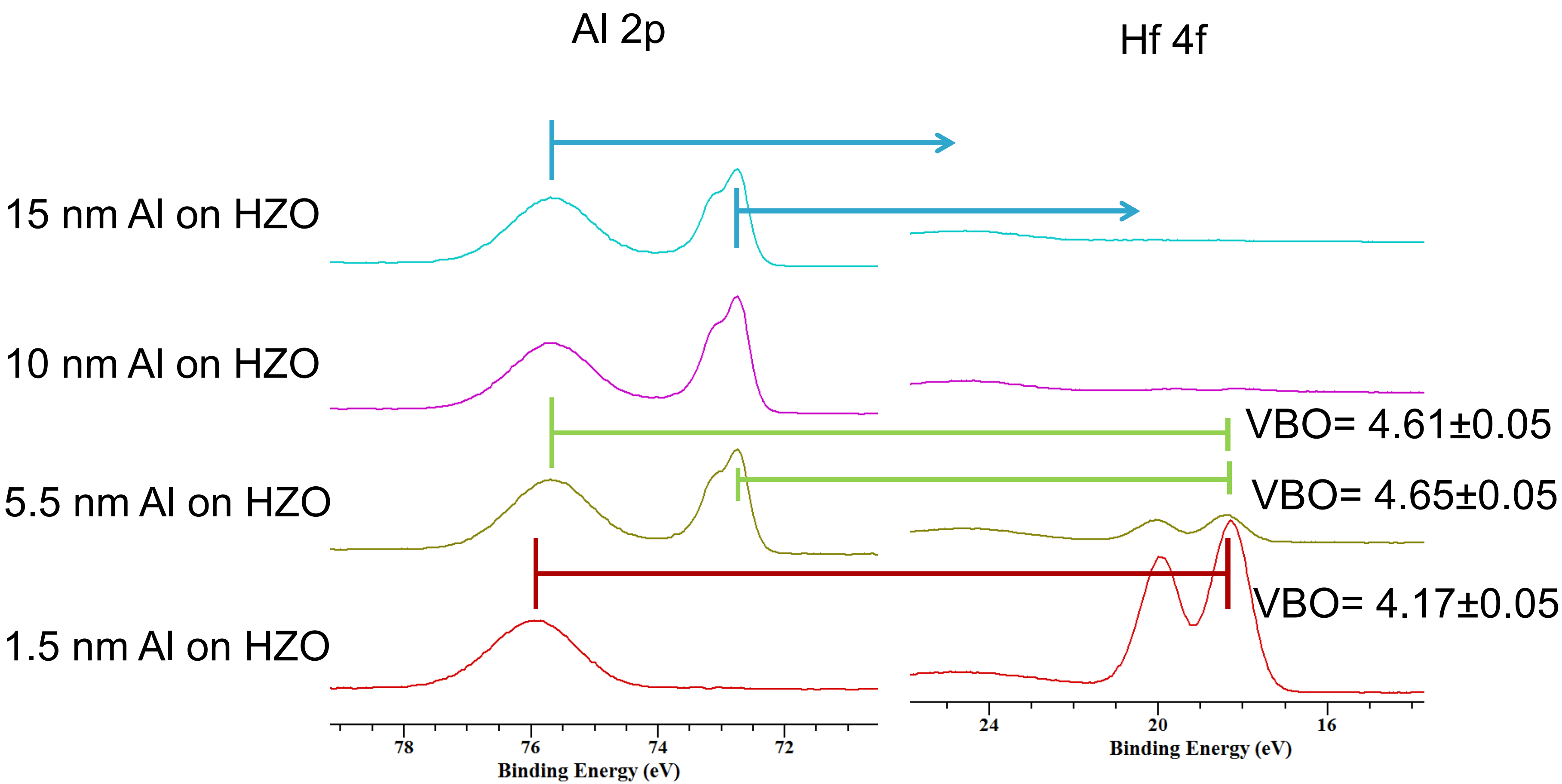
$$VBO = (E_{Ta\ 4f} - E_{VB})^{Ta} + (E_{Zr\ 3d} - E_{Ta\ 4f})^{HZO/Ta} - \mathbf{(E_{Zr\ 3d} - E_{VB})^{HZO}}$$

$$VBO = (E_{Ta\ 4f} - E_{VB})^{Ta} + (E_{Hf\ 4f} - E_{Ta\ 4f})^{HZO/Ta} - \mathbf{(E_{Hf\ 4f} - E_{VB})^{HZO}}$$

For HZO/Ta interface using:
Zr 3d → VBO= 3.24 ± 0.11
Hf 4f → VBO= 3.31 ± 0.10

Mike Brumbach - AVS 2017

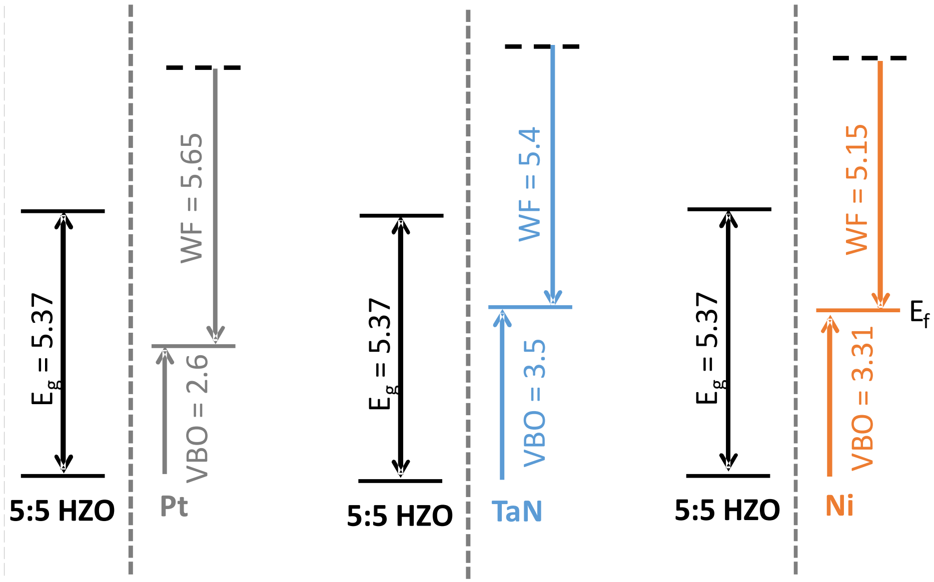
WF combined with VBO
Effect of oxide vs. metal components

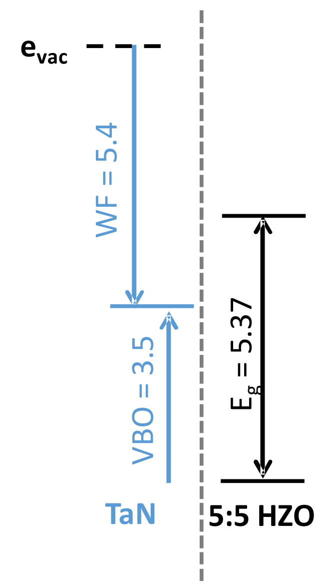


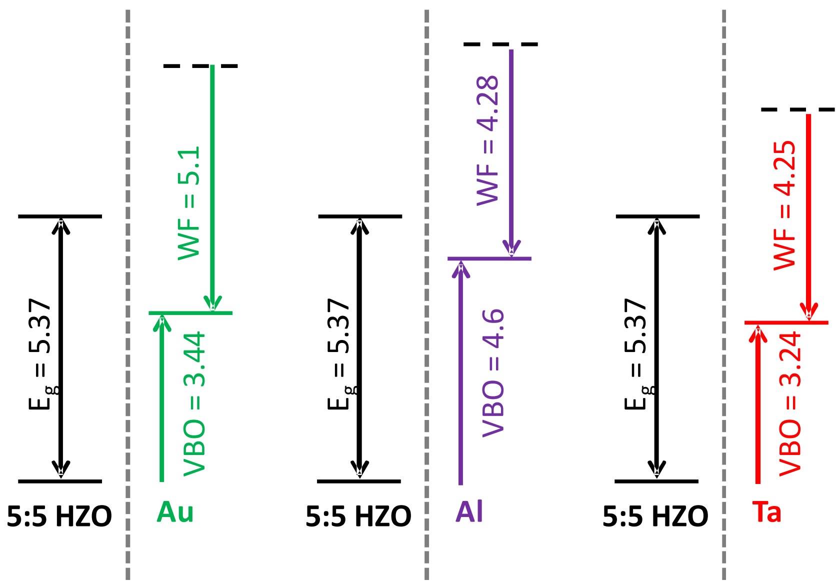
$$VBO = (\mathbf{E}_{\mathit{Al\ 2p}} - E_{VB})^{Al} + (E_{\mathit{Hf\ 4f}} - \mathbf{E}_{\mathit{Al\ 2p}})^{HZO/Al} - (E_{\mathit{Hf\ 4f}} - E_{VB})^{HZO}$$

Standard deviation from measurements at multiple locations.

Relevance to Ferroelectrics







E_g for HZO from Ambriz-Vargaz, et al. APL **110** 093106 (2017)

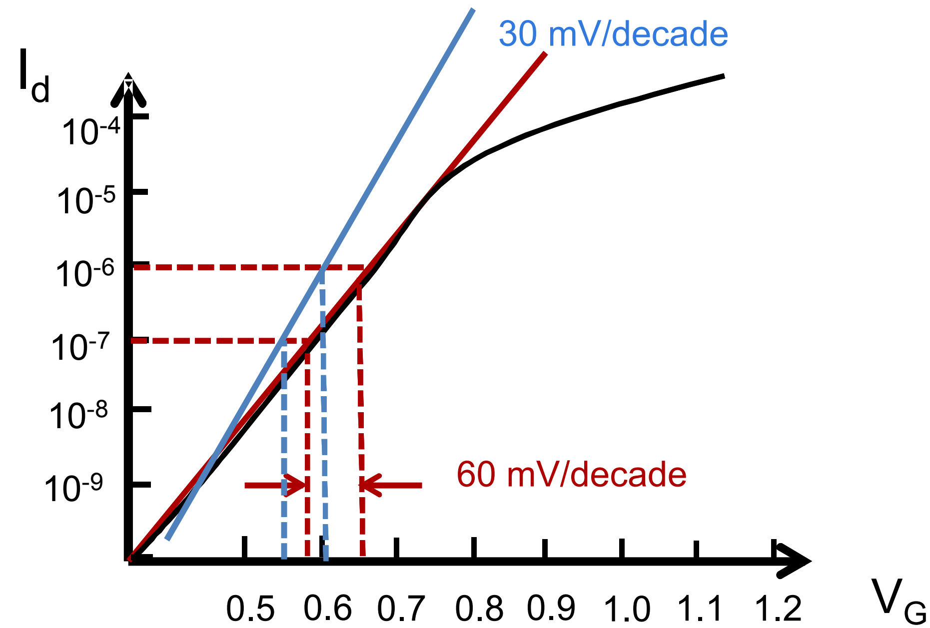
WF for TaN from kelvin probe

WF for gold from literature value (Michaelson, JAP **48** *11* (1977) 4729-4733.)

WF of HZO ~ 4.1 eV

Negative Differential Capacitance

- Negative Differential Capacitance is the idea that by using a ferroelectric in a gate stack, the subthreshold slope can be reduced below the 60mV/decade barrier.
- Experimentally observed in 2015. Tokyo Electronics reported 48 mV/dec using HZO - AVS 2017.



$$S \equiv \frac{\partial V_g}{\partial(\log_{10} I)} = \underbrace{\frac{\partial V_g}{\partial \psi_s}}_{\equiv m} \frac{\partial \psi_s}{\partial(\log_{10} I)} \qquad (1)$$

$$\frac{dV_G}{d\psi_s} = \left(1 + \frac{C_D}{C_{ox}}\right)$$

$$C \simeq \frac{dP}{dE}$$

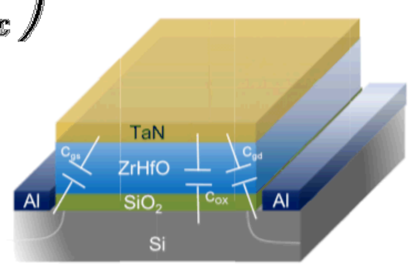
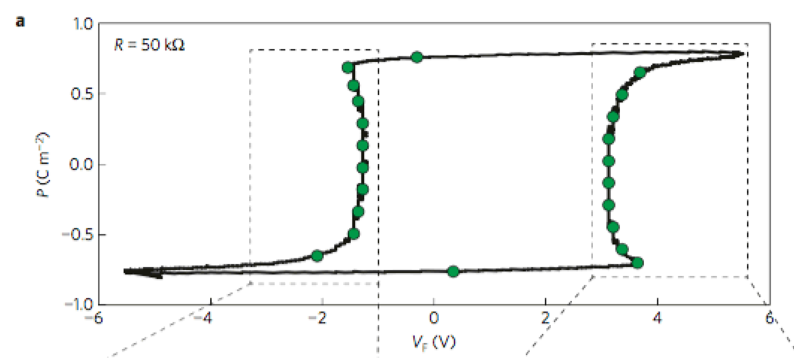


Fig. 1. Schematic structure of low *SS* ZrHfO pMOSFET device.



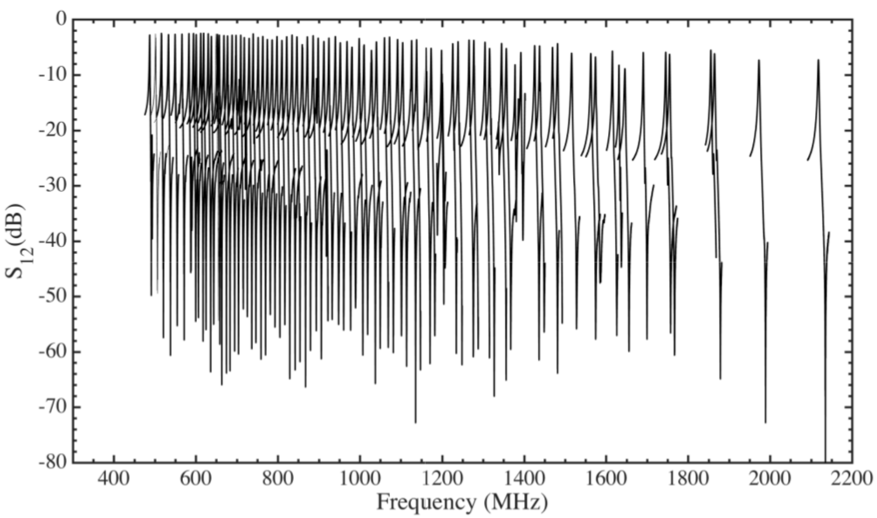
Khan, et al., Nat. Mater., **14** (2015)

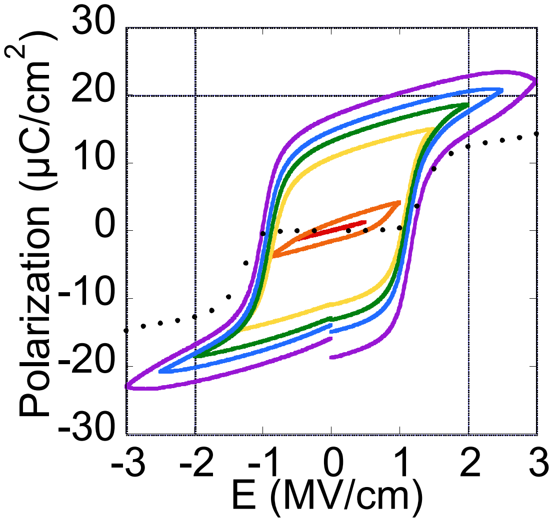
Cheng, et al., IEEE EDL, **35** (2) 2014); Consiglio, S. et al., AVS-Tampa 2017.

Piezoelectric and Ferroelectric for Advance Devices at Sandia MESA Fabrication Facility

Summary

- Development of CMOS compatible piezoelectric films will be essential to develop new technologies:
  - ScAlN is interesting for RF filters but requires a better understanding of microstructure in the film as Sc content increases
  - ALD HZO is looking interesting for dense memory (in close proximity of computational devices) and improved CMOS devices





Piezoelectric and Ferroelectric for Advance Devices at Sandia MESA Fabrication Facility

- ScAlN / AlN Resonator Development

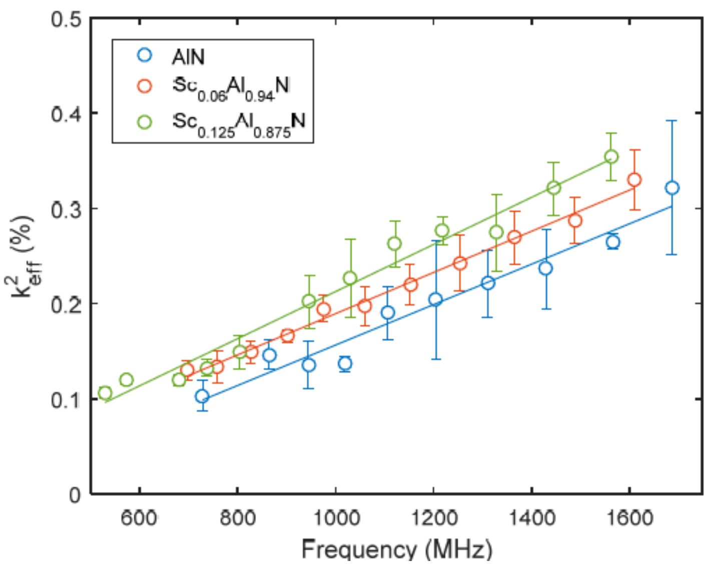
Troy Olsson (DARPA), Ben Griffin, Chris Nordquist, Aleem Siddiqi, Peggy Clews, Erica Douglas, Matt Eichenfield, Giovanni Esteves, Travis Young, Bob Timon, David Adams, lots and lots more.

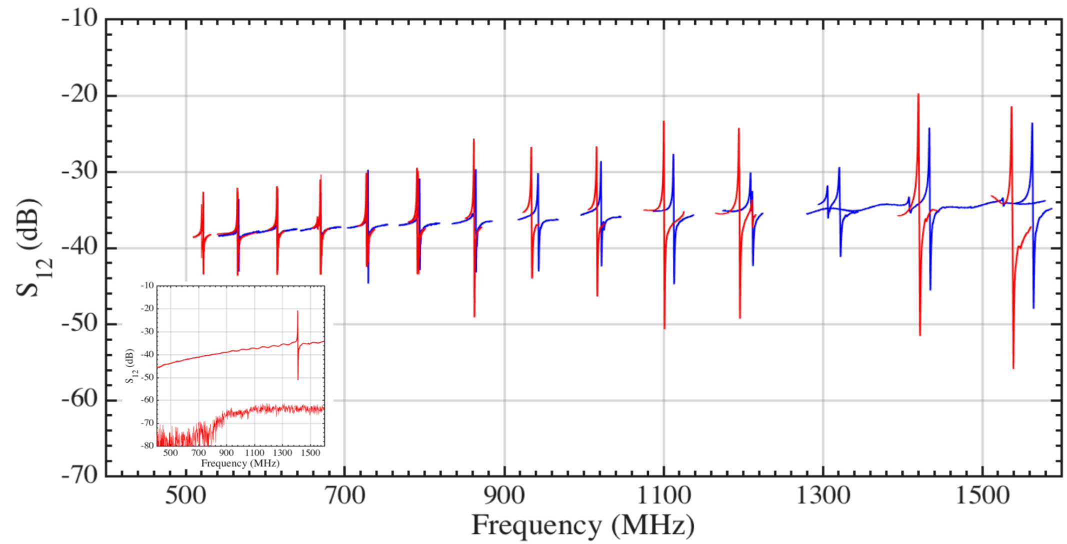
- HfZrOx Development

Jon Ihlefeld (UVa), Sean Smith, Mike Brumbach, Travis Young, Paul Davids, lots and lots more.

Fabrication was performed at Sandia's MESA Fab facility and we gratefully acknowledge all their work.

Top Metal IDT CMR 6% ScAlN Performance





Red is the ScAlN resonators and blue is AlN. A clear improvement in resonator Q and k^2_{eff} is visible.

Measured acoustic velocity in ScAlN = 9860 m/sec.