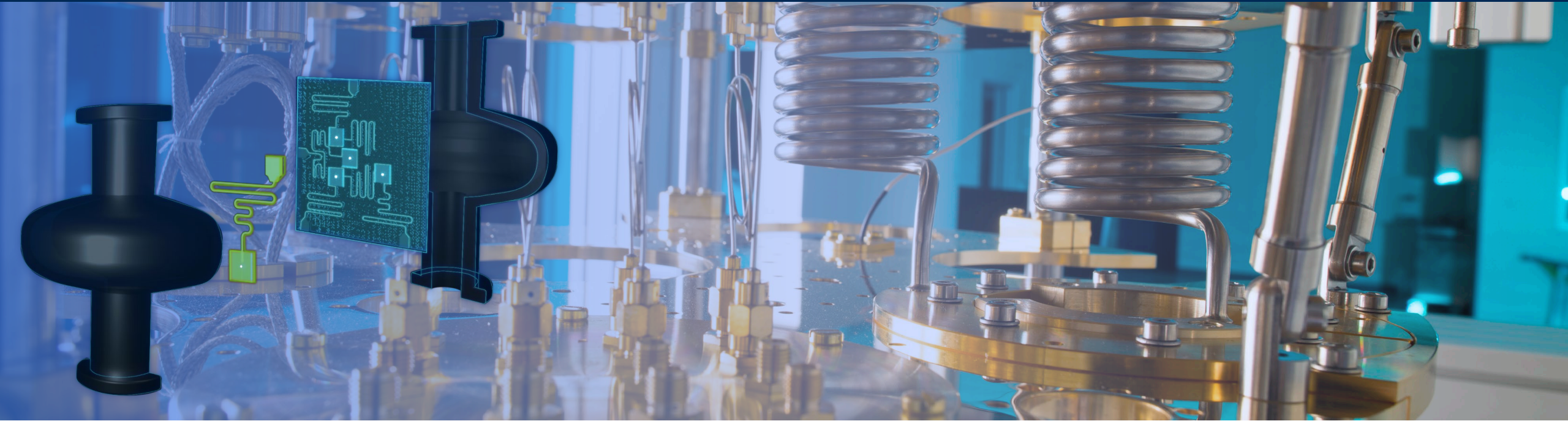


# Report Pillar1 SQMS

Angelo

SMQS Italia 15-16 Dicembre 2022



# Understanding and Mitigating Decoherence in Superconducting Quantum Devices & Sensors: *Pillar 1*

Alex Romanenko

Matt Kramer

Jens Kock

10/18/2022

# How can better fabrication make a better quantum computer?

## Known sources of decoherence

- Charge/flux noise
- Quasi-particles
- TLS/Dielectric loss

## Potential solutions

- Transmon, 3D Transmon
- Fluxonium, 0-Pi, etc
- Better design, filtering, shielding
- Lower loss material and interfaces

What appendix 13 activity and/or WBS deliverable do these activities address?

## Challenge to address:

- Identify, characterize, and mitigate sources of RF loss that limit the performance of 2-D and 3-D structures quantum structures

## Cross Cutting Activities:

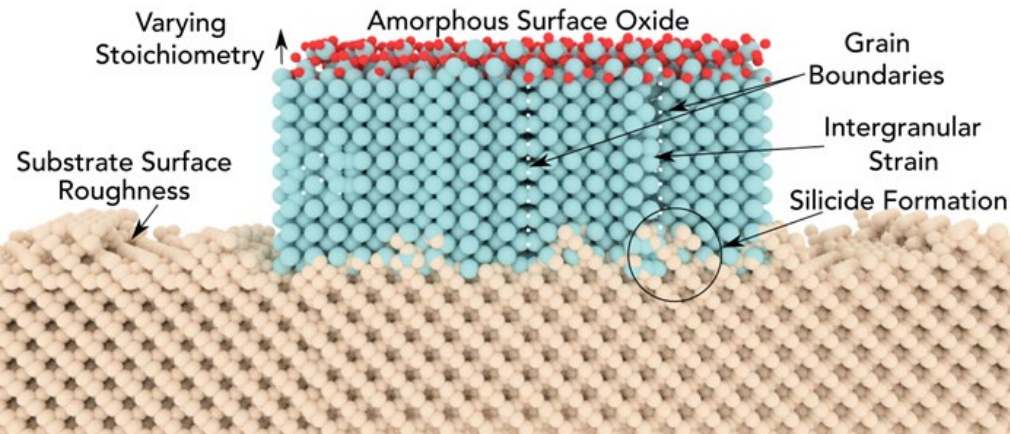
- Touches all major activities delineated in App 13

Focus Area	Major Activity	Deliverables and Benchmarks	Center Year				
			1	2	3	4	5
Materials for 2D and 3D Quantum Devices	(1) Infrastructure & Testbeds <i>Impacts: (2), (3), (4), (5).</i>	Infrastructure upgrades to enable low (T~1.5K) and ultralow (T<=100mK) temperature characterization stations at partner institutions <i>*Risk mitigation: risk reduction via creation of additional testing bandwidth to evaluate new ideas</i>					
		SRF cavity-based testbed available for characterizing dielectrics in quantum regime at Fermilab					
		SRF cavity-based testbed available for characterizing dielectrics in the quantum regime at Northwestern and NIST/UCorlando					
	(2) Advanced Materials Studies	Initial exploration of dominant quasiparticle sources including underground measurements (INFN) of the 2D Rigetti transmon <i>*Risk mitigation: by testing the same devices in different testbeds by different experimenters, environments and techniques that maximize performance can be identified</i>					
	<i>Impacts: (4), (5)</i> <i>Drives: (1)</i>	Measuring loss tangents of (several kinds of) Si and sapphire in the quantum regime inside the high Q SRF cavity <i>*Risk mitigation: explore both silicon and sapphire to down-select to lowest-loss substrate</i>					
		Spectroscopic and superconducting properties investigations of Nb and Al in the full quantum regime (e.g., penetration depth, STM, STS)					
		Cryogenic structural investigations of 2D transmons and SRF cavity cutouts (e.g., FIB, TEM, AFM, MFM) <i>*Risk mitigation: continue advanced materials studies throughout program for continued progress in materials development and as means to troubleshoot problems that develop</i>					
		Devise techniques of minimizing surface magnetic moments in substrate materials via theoretical and experimental effort					
	(3) Two Level Systems and Surface Passivation <i>Impacts: (4), (5)</i> <i>Drives: (1)</i>	Identify theoretically and experimentally best techniques for comprehensive interface characterization and initial loss mitigation for TLSs					
		Several candidates for TLS based on detailed comparative structural studies of "bad" vs "good" transmons					
		Exploring niobium passivation techniques compatible with SRF cavities					
		Exploring niobium/aluminum oxide removal and passivation techniques compatible with 2D transmons <i>*Risk mitigation: by studying TLS reduction and surface passivation in both 2D and 3D structures, lessons learned can be transferred between groups</i>					
		Develop an atomic-level mechanistic understanding of TLSs					
	(4) Transmon Coherence Time Milestones <i>Impacts: (6), (7), (10), (13), (14)</i> <i>Drives: (1)</i>	Modified manufacturing procedures and/or post-manufacturing treatments of 2D superconducting transmons to achieve maximum individual coherence times > 1 ms					
		Delineate specifications for bulk substrate materials to ensure coherence of transmon > 1 ms with spread < 20%					
		Modify manufacturing procedures and/or post-manufacturing treatments of 2D superconducting transmons to achieve coherence times > 1 ms with less than 20% spread					
	(5) 3D Resonator Performance Milestones <i>Impacts: (6), (10), (11), (12), (13), (14)</i> <i>Drives: (1), (2), (3)</i>	Demonstration of high Q FNAL-Rigetti coupled SRF cavity-transmon system					
		Demonstrate individual SRF cavities of > 5 sec coherence times in the quantum regime					
		Demonstrate advanced performance metrics for integrated cavity-transmon systems					
		Demonstrate robust treatments to preserve Q > 1e11 and photon lifetimes > 10 seconds in SRF cavities that are insensitive to air exposure					



# Summary of 10/18/2022 discussion

## Nanoscale Sources of Decoherence



**Performance of 2D quantum devices and 3D cavities: decoherence characterization, understanding, mitigation**

Josh Mutus, Daniel Bafia, Shaojiang Zhu

**Materials characterization**

Akshay Murthy, Lin Zhou, Michael Bedzyk

**Device Design and Fabrication**

Mustafa Bal, Florent Lecocq, Yuvraj Mohan

**Device Design and Fabrication**

Mustafa Bal, Florent Lecocq, Yuvraj Mohan

**Superconducting properties characterization and theory**

Maria Iavarone, Venkat Chandrasekhar, Jim Sauls

SQMS	Thrust	Focus Area	Major Activity	Deliverables	Project Leader
1.1	Technology	1.1.1	Materials for 2D and 3D Devices		
		1.1.1.1	Infrastructure and Testbeds		
			1.1.1.1.1 Prepare low temp infrastructure upgrades - characterization stations		Alex/Akshay
			1.1.1.1.2 Prepare Quantum Computing Lab - 2		Sam Posen, Olek Melnychuk
			1.1.1.1.3 Prepare Quantum Computing Lab - 3		Roman, Daniil
			1.1.1.1.4 Nanofabrication Testbed		Mustafa
			1.1.1.1.5 Prepare SRF Cavity-based testbed at FNAL for quantum material characterization		Mattia
			1.1.1.1.6 Prepare infrastructure for standardized 3D transmon characterization across different institutions		Anna, Jim Sauls
			1.1.1.1.7 Round Robin		Josh Mutus
		1.1.1.2	Fabrication		Bal/Grassellino
			1.1.1.2.1 Nb/air interface		
			1.1.1.2.2 Nb/substrate interface		
			1.1.1.2.3 Superconductor		
			1.1.1.2.4 Josephson junction		
		1.1.1.3	Characterization		
			1.1.1.3.1 Nb/air interface		
			1.1.1.3.2 Nb/substrate interface		
			1.1.1.3.3 Superconductor		
			1.1.1.3.4 Josephson junction		
		1.1.1.4	Theory/Simulation		
			1.1.1.4.1 Nb/air interface		
			1.1.1.4.2 Nb/substrate interface		
			1.1.1.4.3 Superconductor		
			1.1.1.4.4 Josephson junction		
			1.1.1.4.5 Device model		

Major new focus this year

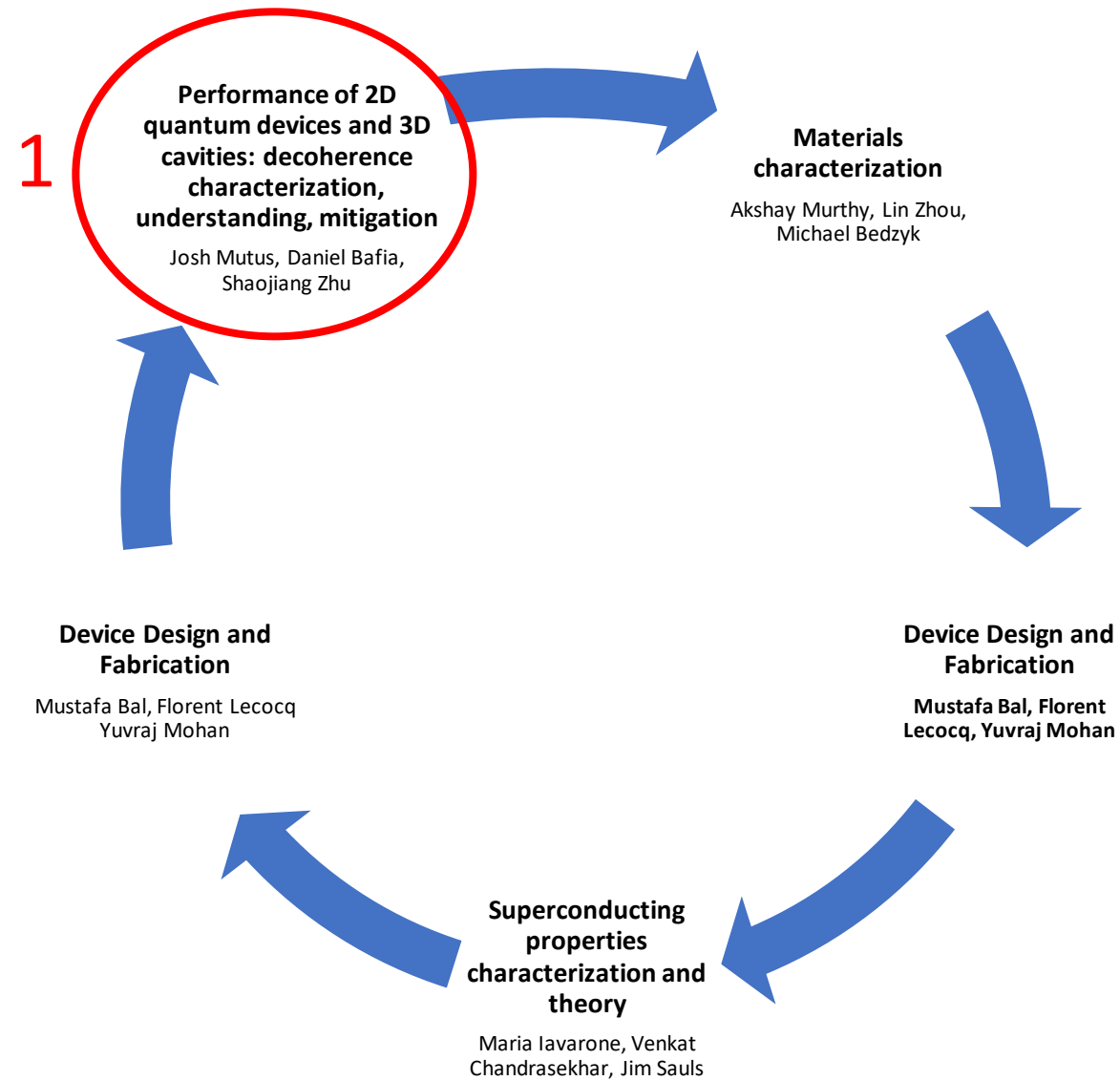
Adoption of improved Materials and processes

# Key Areas and Unknowns

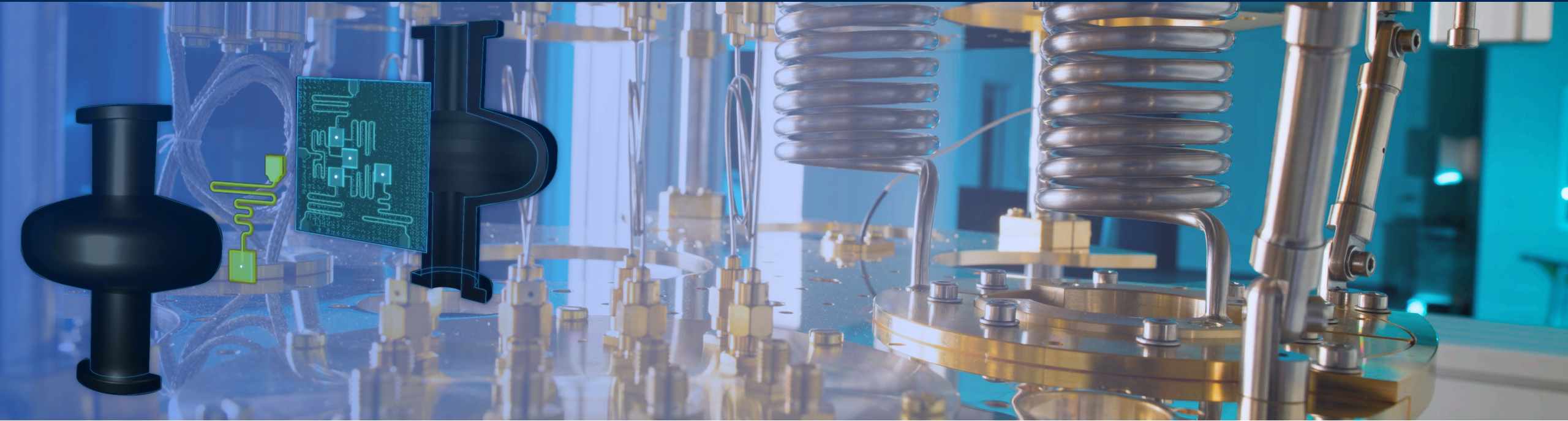
- Performance of 2D/3D transmons
  - Where are the losses coming from and do we know what fraction of the losses are coming from which components?
- SC components
  - Nb-O is the source for major losses, bulk as well in the film. This is well confirmed for SRF cavities, but not as clear for the 2D transmons.
  - Al JJ's were not discussed much, but there are questions about the defects associated with the deposition rates, etching and lift-out processing.
  - What losses are coming from the Nb and what is coming from JJ's. Losses with the Al may also be dependent on the filtering during testing.

# Key Areas and Unknowns

- Substrates
  - Si losses are 10x worse than expected.
  - Sapphire is not as good as expected, are there better materials (dielectrics)?
    - Quality variation may be dependent on where the materials were sourced from. Quality of the Nb on sapphire appears to be better, but what about the superconducting properties?
- Processing
  - Is there a way of getting a clean measurement without breaking vacuum (IBM tried this)
  - We are looking at several ways of encapsulating the Nb? What is most effective? What methods can we quickly bring to bear to more quickly determine which is most promising? Are what works for cavities most relevant for thin films or is something else dominating decoherence?







# Performance of 2D Quantum Devices and 3D Cavities: Decoherence Characterization, Understanding, Mitigation

Josh Mutus

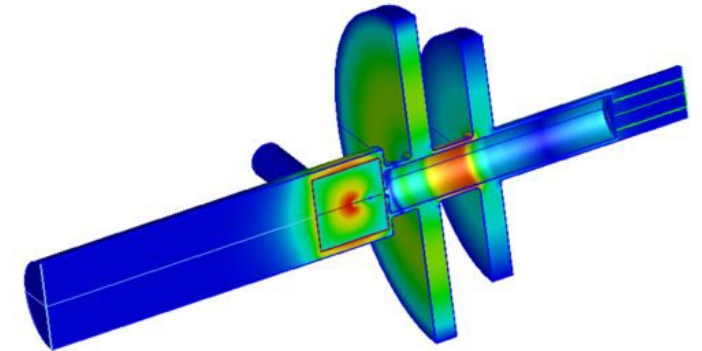
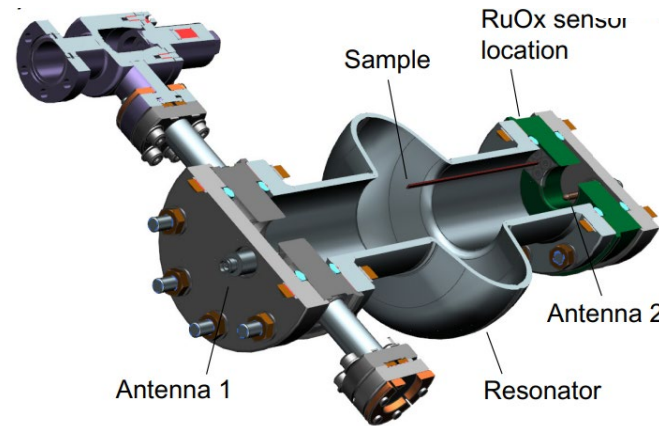
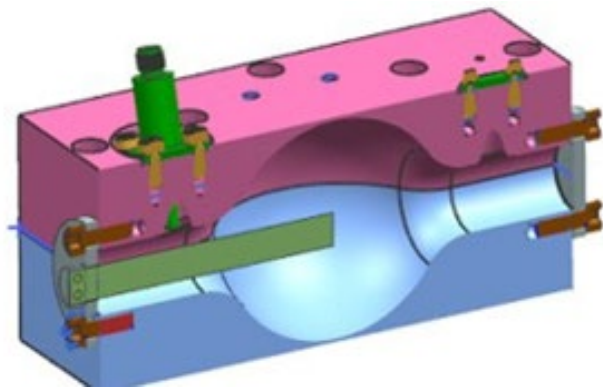
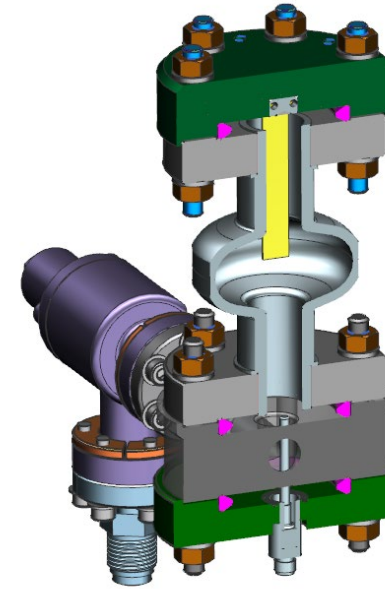
Daniel Bafia

Shaojiang Zhu

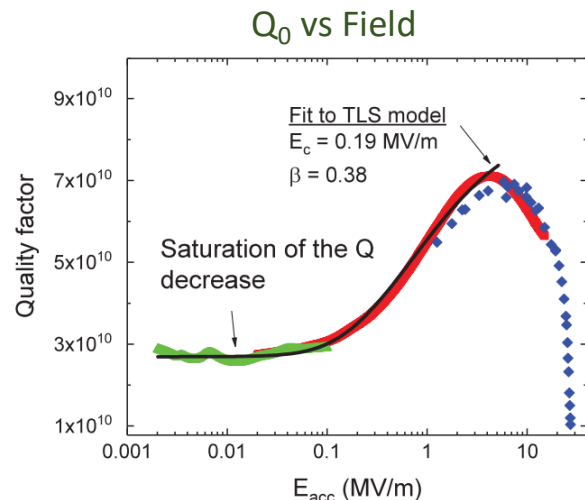
11/18/2022

# What 3-D devices are we using to identify sources of decoherence?

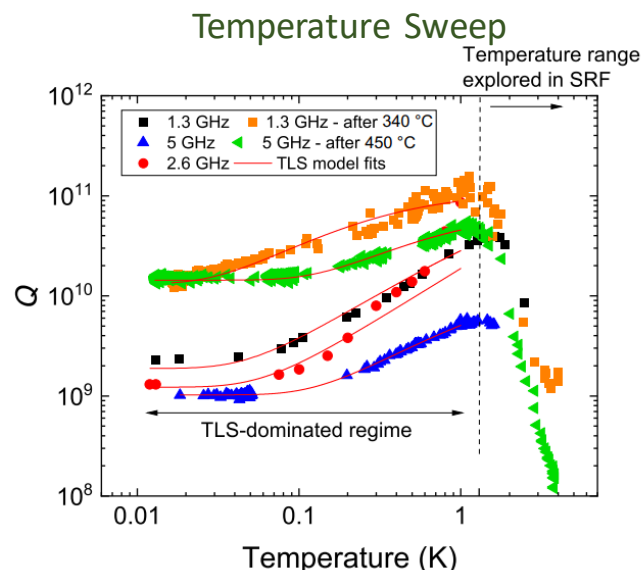
- Built up cavity testbed at FNAL to enable RF measurements on a variety of materials
  - 6x 6 GHz bulk Nb cavities
  - 2x 2.6 GHz bulk Nb cavities
  - 2x 5 GHz bulk aluminum cavities
  - 1x Tunable cavity



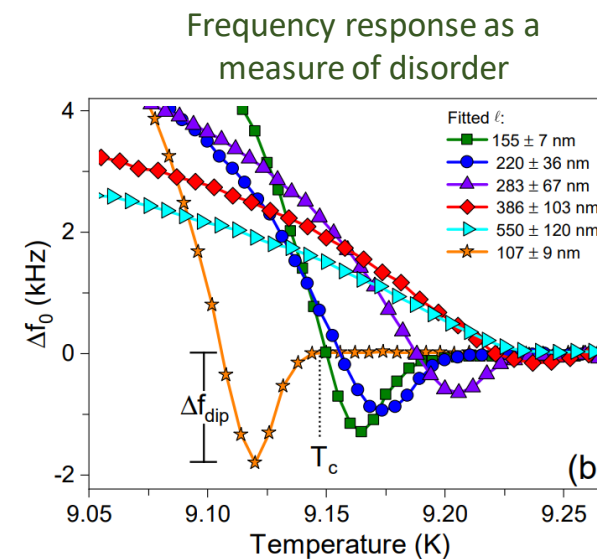
# What 3-D resonator techniques are we using to characterize sources of decoherences?



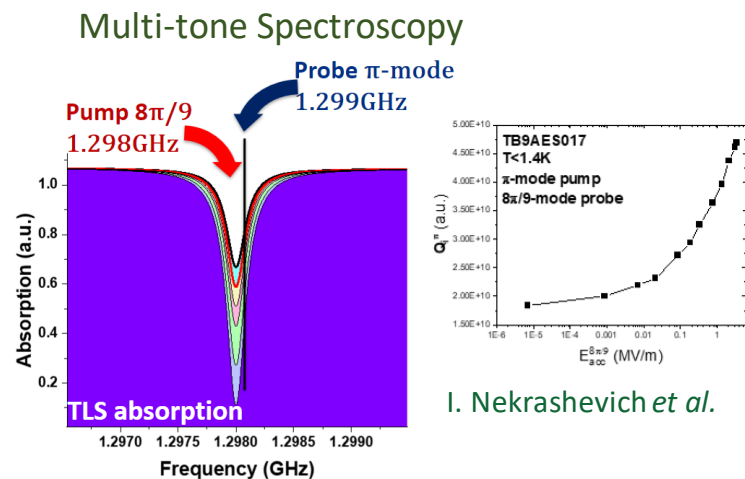
A. Romanenko D. Schuster., PRL **119**, 264801 (2017)



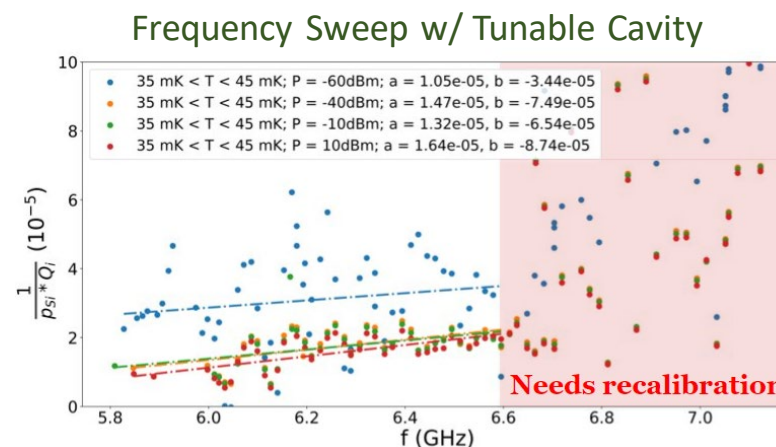
A. Romanenko *et al.*, PRAppl **13**, 034032 (2020)



D. Bafia *et al.* [arXiv:2103.10601](https://arxiv.org/abs/2103.10601)



I. Nekrashevich *et al.*



I. Nekrashevich *et al.*



# Most sensitive measurement of niobium oxide loss tangent at mK and demonstrating photon lifetimes of 2 s in Nb SRF cavities

A. Romanenko, R. Pilipenko, S. Zorzetti D. Frolov, M. Awida, S. Belomestnykh, S. Posen, and A. Grassellino, PRAppl **13**, 034032 (2020)

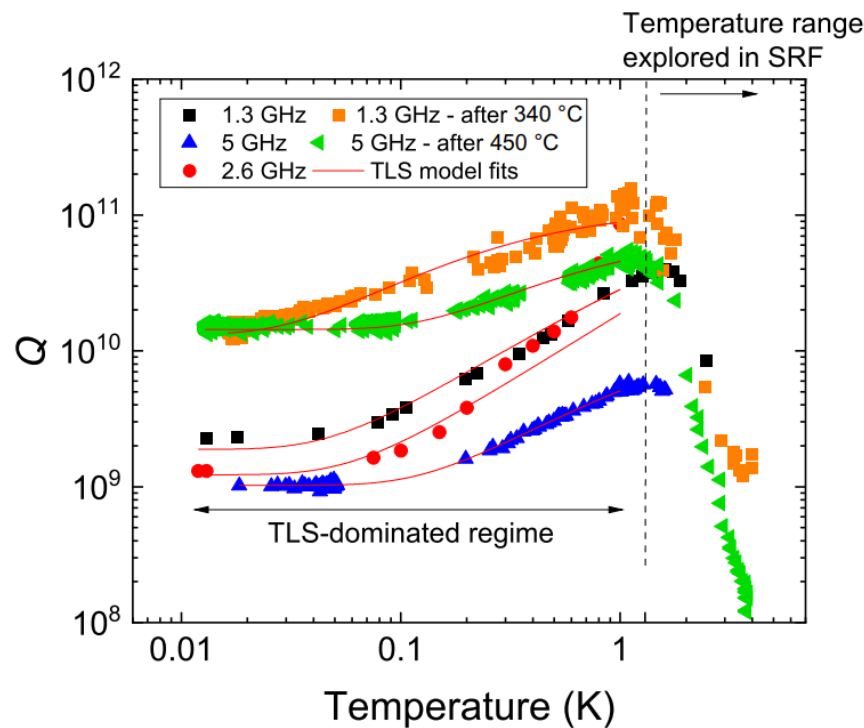


TABLE I. Summary of TLS model fitting results.

$f_0$ (GHz)	Oxide treatment	$F\delta_0$	$F$	$\delta_0$
1.3	No	$5.2 \times 10^{-10}$	$1.0 \times 10^{-7}$	0.17
2.6	No	$8.2 \times 10^{-10}$	$2.4 \times 10^{-8}$	0.13
5	No	$9.1 \times 10^{-10}$	$1.2 \times 10^{-8}$	0.08
1.3	340°C 3 h	$6.7 \times 10^{-11}$	...	...
5	450°C 3 h	$5.6 \times 10^{-11}$	...	...

## Scientific Achievement

Obtained most sensitive measure of the niobium oxide dielectric loss tangent using bulk niobium SRF cavities. Eliminating the oxide *via* vacuum baking yielded record photon lifetimes.

## Significance and Impact

These results identify the native niobium oxide as a major source of decoherence in 2-D transmons and 3-D cavities used in the quantum regime. These findings motivate material studies to identify treatments which make cavities and 2-D devices robust against air exposure.

## Details

- 3 cavities of various resonant frequencies were tested before and after *in situ* vacuum baking treatments which removed the oxide
- Cavities were tested from ~2 K down to ~20 mK at single photon levels
- RF data was fitted with standard-TLS model

# Most sensitive measurement of silicon loss tangent at mK temperatures

M. Checchin, D. Frolov, A. Lunin, A. Grassellino, and A. Romanenko,  
PRApplied **18**, 034013 (2022)

## Scientific Achievement

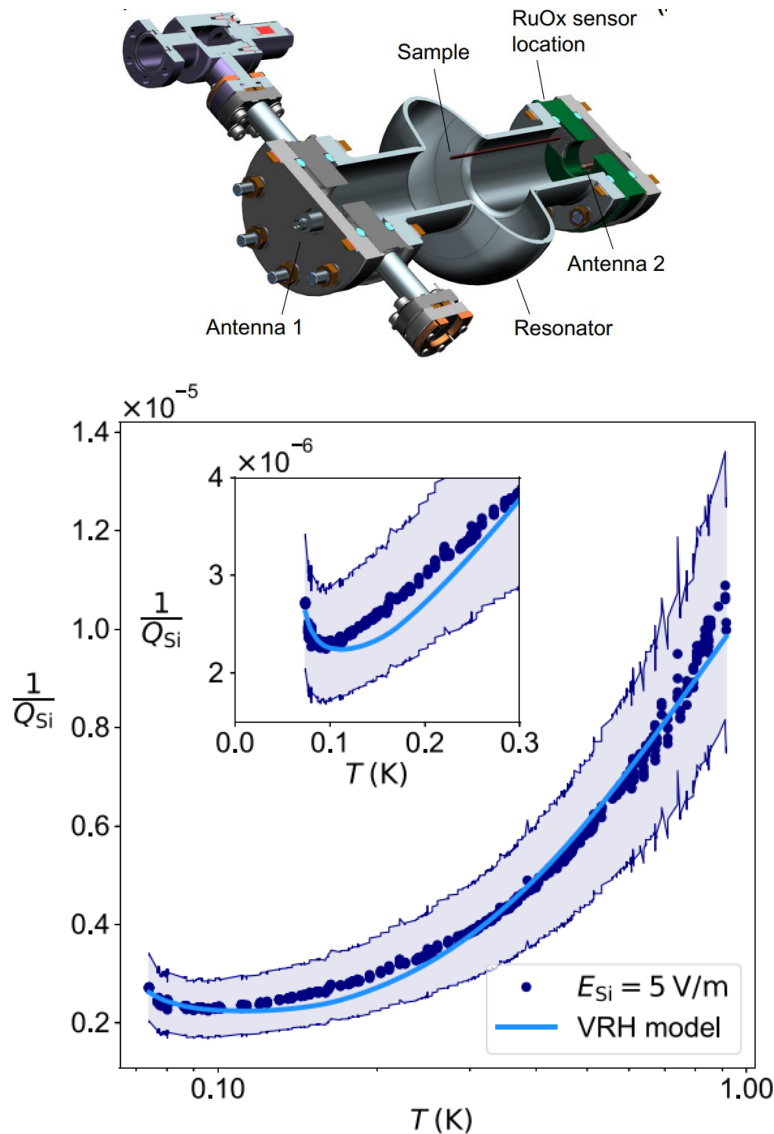
Measured loss tangent of high resistivity intrinsic FZ (100) at fields and temperatures commonly used for planar transmon device operation and found that the values are 10X greater than previous measurements

## Significance and Impact

These results suggest that the above substrate is a potentially dramatic source of decoherence in 2-D transmon devices, limiting coherence times to ~50 us.

## Details

- A 2.6 GHz cavity Nb cavity was loaded with a 10 k $\Omega$  cm FZ intrinsic (100) Si samples with dimensions of 100 mm x 2 mm x .675 mm
- Integrated setup measured in a DR down to ~70 mK and down to field levels which correspond to intra-cavity photon number of  $\sim 10^8$
- Resulting data showed Si loss tangents of 2e-6, 10x higher than previous measurements
- Non-monotonic dependence of loss tangent with temperature likely due to variable range conductivity – highlights conductive losses in Si



# Measure loss tangent of several kinds of Si and sapphire and delineate specs which ensure coherence >1ms

	Impacts: (4),(5) Drives: (1)	Measuring loss tangents of (several kinds of) Si and sapphire in the quantum regime inside the high Q SRF cavity <i>*Risk mitigation: explore both silicon and sapphire to down-select to lowest-loss substrate</i>					
		Spectroscopic and superconducting properties investigations of Nb and Al in the full quantum regime (e.g., penetration depth, STM, STS)					
		Cryogenic structural investigations of 2D transmons and SRF cavity cutouts (e.g., FIB, TEM, AFM, MFM) <i>*Risk mitigation: continue advanced materials studies throughout program for continued progress in materials development and as means to troubleshoot problems that develop</i>					
		Devise techniques of minimizing surface magnetic moments in substrate materials via theoretical and experimental effort					

	(4) Transmon Coherence Time Milestones Impacts: (6),(7), (10),(13),(14) Drives: (1)	Modified manufacturing procedures and/or post-manufacturing treatments of 2D superconducting transmons to achieve maximum individual coherence times > 1 ms					
		Delineate specifications for bulk substrate materials to ensure coherence of transmon > 1 ms with spread < 20%					
		Modify manufacturing procedures and/or post-manufacturing treatments of 2D superconducting transmons to achieve coherence times > 1 ms with less than 20% spread					

Current status: measured one Si sample and currently measuring sapphire

Next steps:

- Ramp up Si substrate RF studies
  - Samples already procured, cavities ready, just need DR time
- Ramp up sapphire substrate RF studies:
  - Compare vendors, orientations, ...
- Collaborate with other institutions and test reproducibility (like RR)

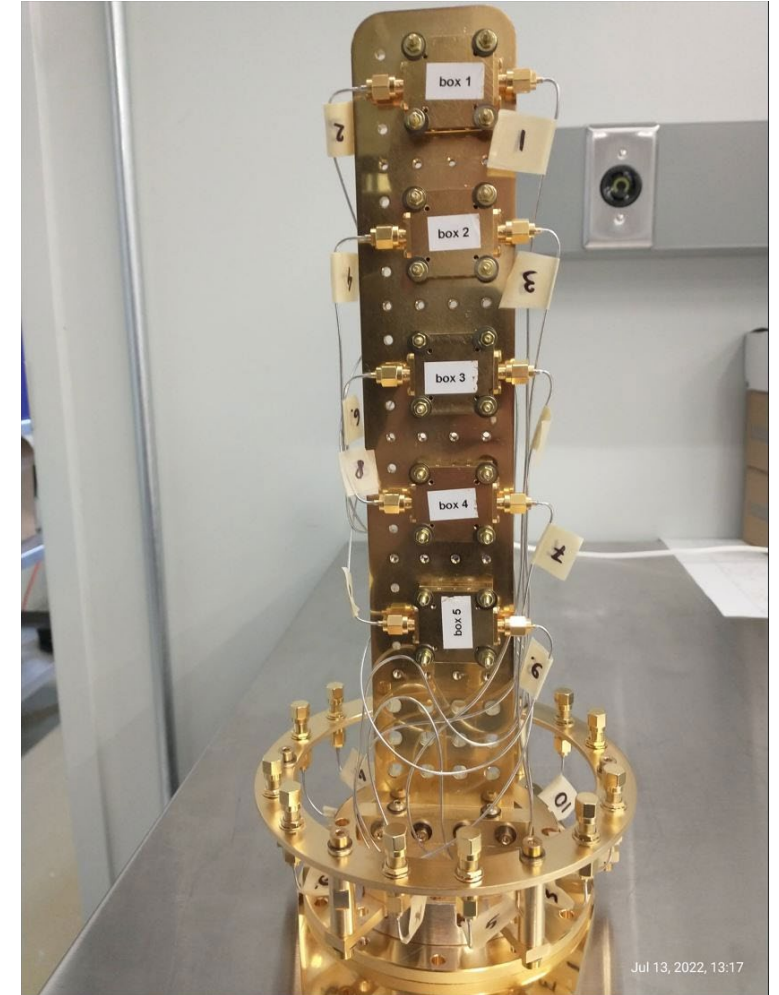
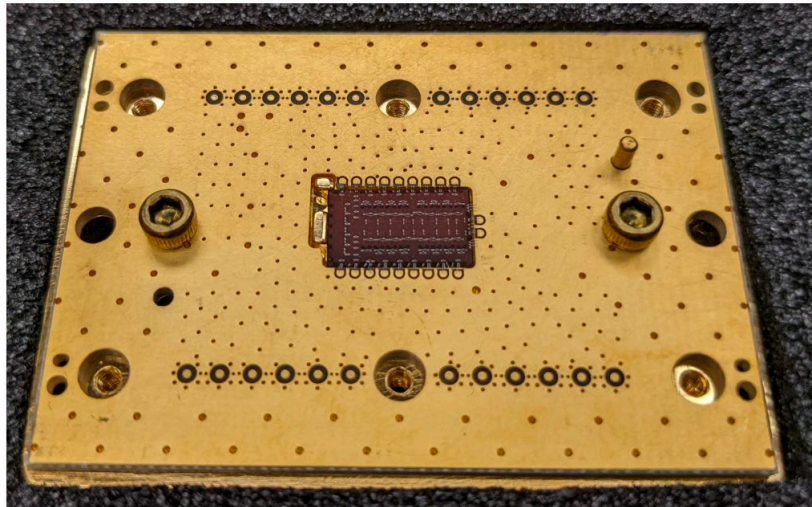
Si substrate parameter sweep

Resistivity [kΩ cm]	10	30	50
Oxide Removal			
Surface Roughness (SSP vs DSP)			
Dopants			
Orientations (100 vs 111, etc)			



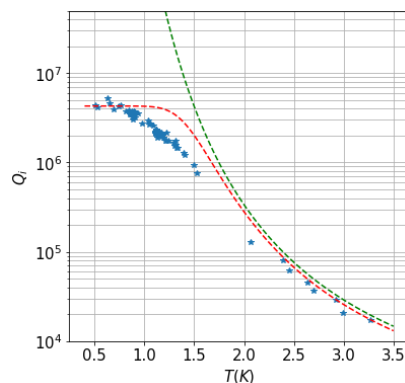
# What 2D devices are we using to identify sources of decoherence?

- Planar Qubits
  - SQMS Standard (8 fixed frequency)
  - Round Robin (14 tunable, 2 fixed)
- Planar Resonators
  - SQMS varied geometry
  - SQMS metal-substrate targeting geometry



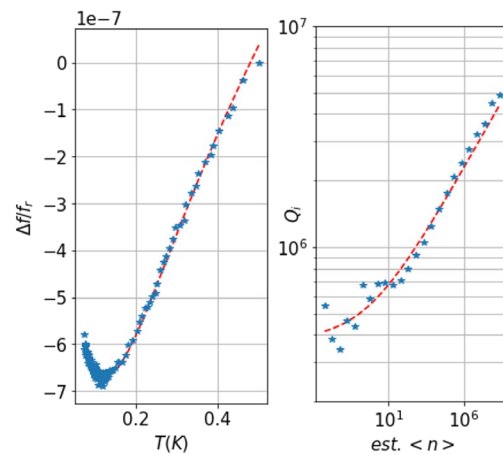
# What 2D resonator techniques are we using to characterize sources of decoherences?

$Q_i$  vs Power



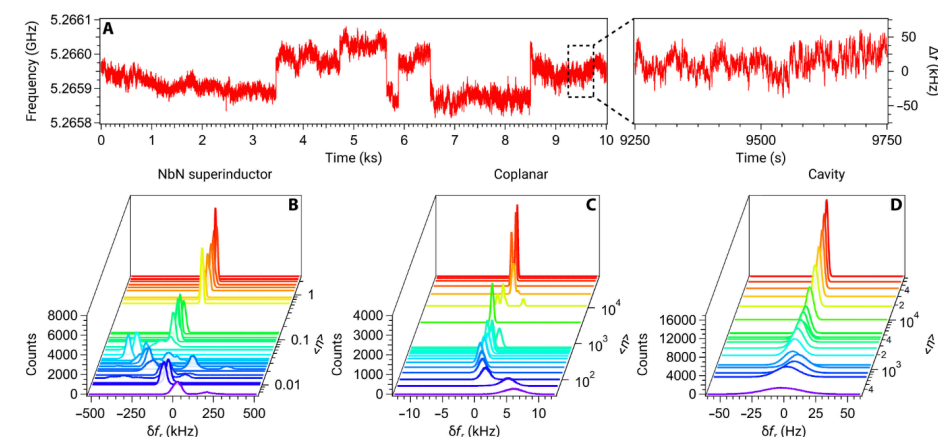
A. Romanenko D. Schuster., PRL **119**, 264801 (2017)

$Q_i$  and  $f_o$  vs Temperature



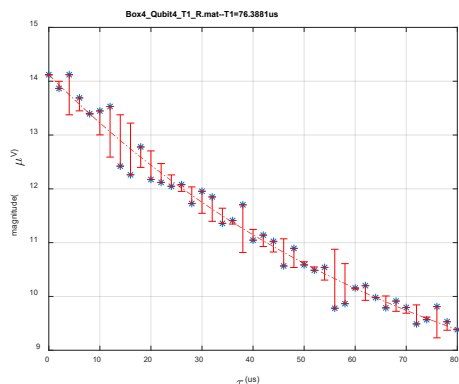
A. Romanenko *et al.*, PRAppI **13**, 034032 (2020)

Time dependence of  $Q_i$  and  $f_o$

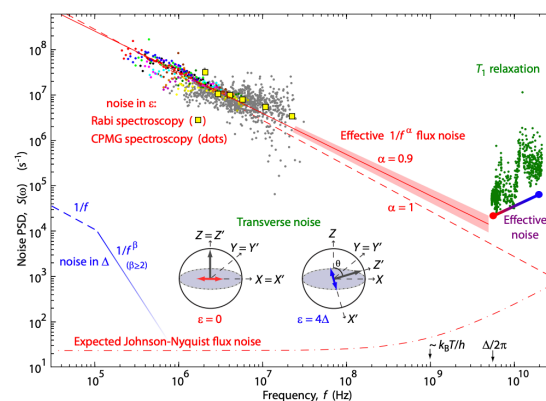


<https://www.science.org/doi/10.1126/sciadv.abh0462>

$T_1$ ,  $T_2$ ,  $T_2^*$ ,  $P_1$  vs Time, Temperature

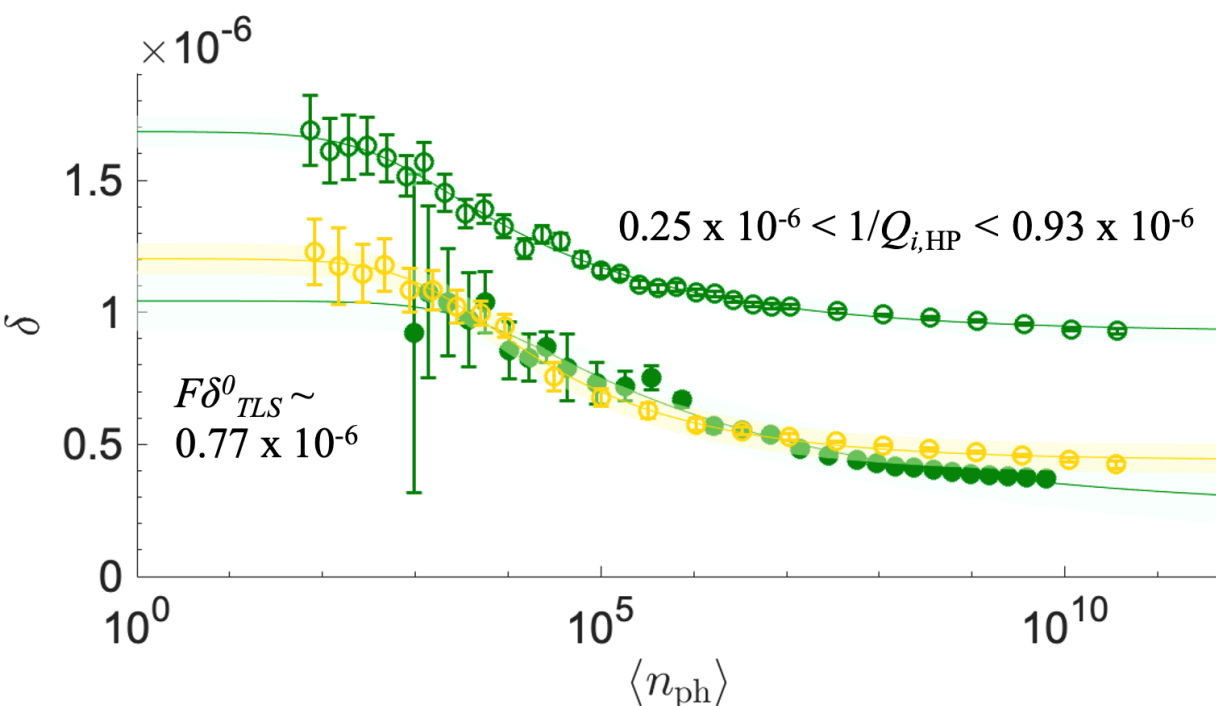


\*PSD of qubit noise DD, CPMG



<https://arxiv.org/abs/1101.4707>

# Reproducible Measurement of TLS Loss in a Nb on Si Resonator



Loss  $\delta$  as a function of estimated average number of photons in the resonator  $\langle n_{ph} \rangle$  for resonators at  $f_0 = 5.532$  GHz (green) and  $f_0 = 5.066$  GHz (yellow). Open markers: CU Boulder at  $T \sim 11$  mK. Closed markers: NIST at  $T \sim 35$  mK. Markers are shown with error bars indicating a 95% confidence interval for the  $Q_i$  fit using the scresonators Python package. Solid lines: least squares fit to the TLS model. Shaded region: 95% confidence band.

## Scientific Achievement:

Demonstrated reproducible measurement of effective TLS loss with precision  $< 10\%$  across two SQMS measurement sites (CU and NIST)

## Significance and Impact:

This demonstrates a preliminary step towards leveraging the distributed measurement power of the SQMS Center.

## Details

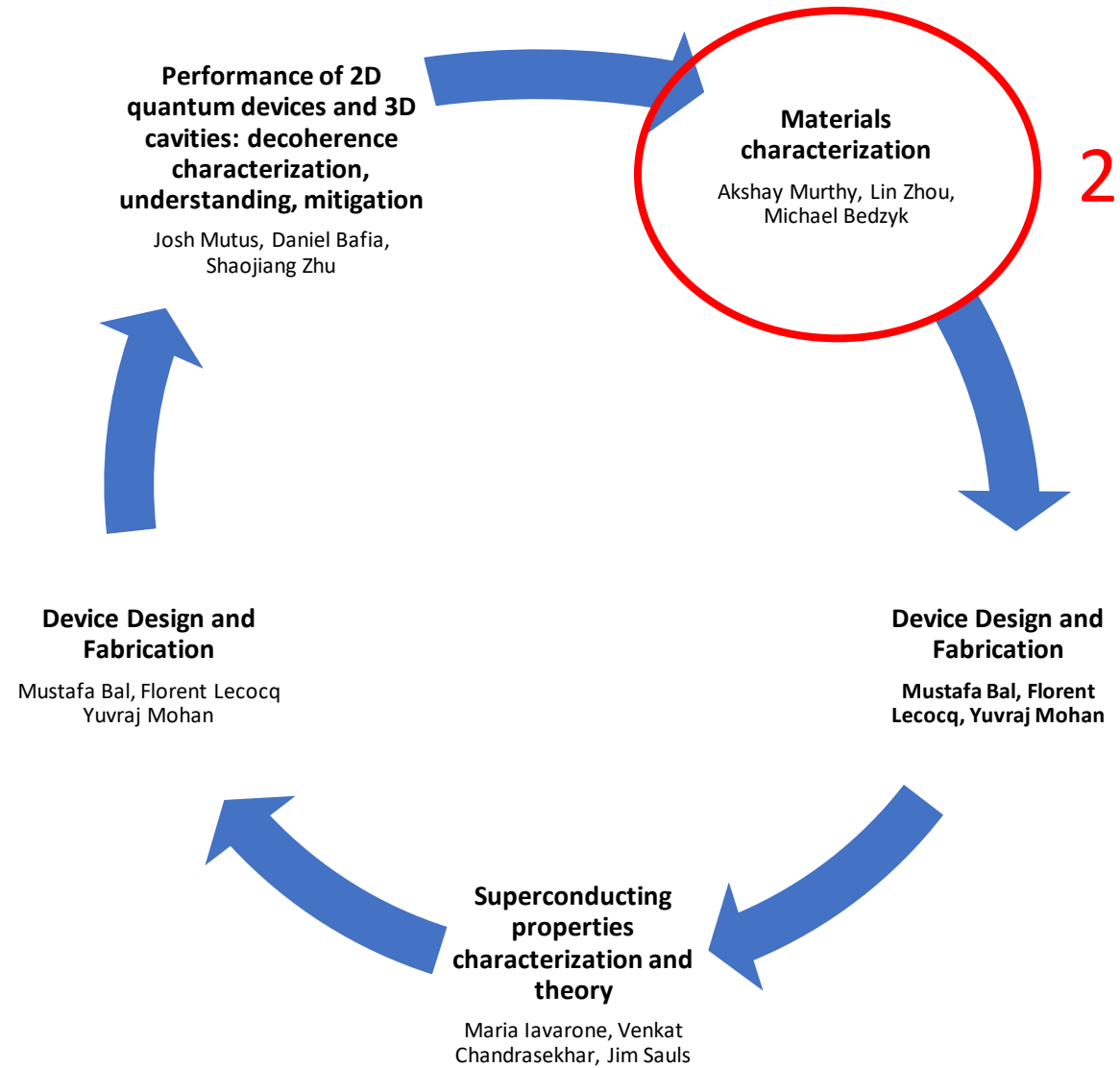
See [Corey Rae McRae's poster at the SQMS Poster Session](#) for more details.

## For 2D devices: What still needs to be done by the time of the technical review?

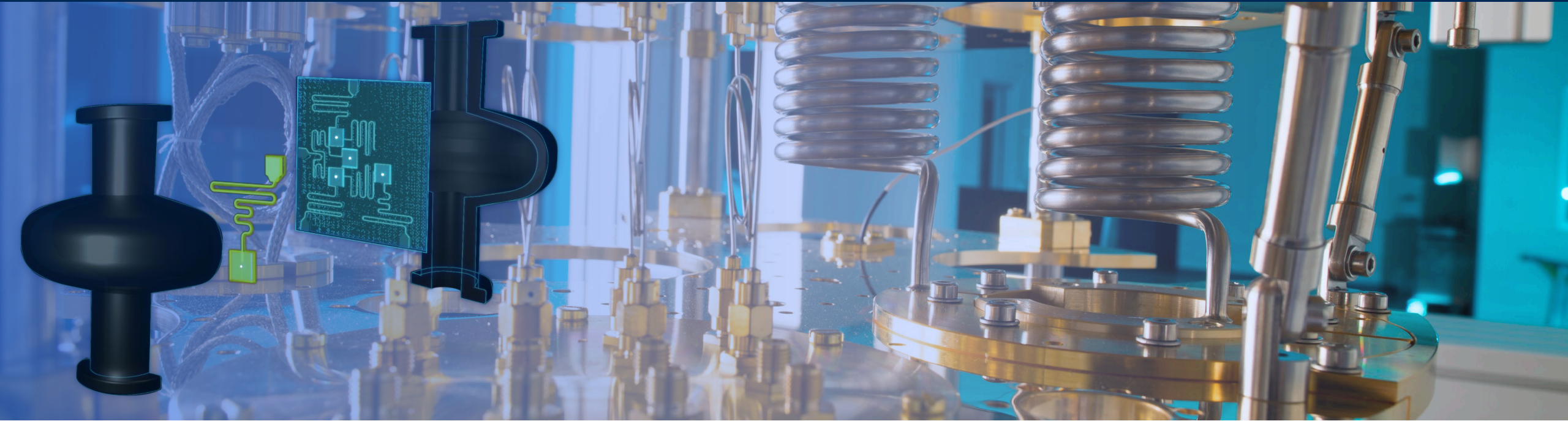
- **(P0) Fabricate and characterize devices on bi-layer encapsulating materials from NIST, FNAL, NU and Rigetti**
- Perform noise characterization experiments at SQMS, CPMG etc
- Connect QP theory with device experiments
- Iterate on SQMS resonator masks for coverage of interfaces

# What still needs to be done to reach Appendix 13 deliverable? What are the long term goals?

- Primary bottleneck: getting DR time
  - Multiple experiments can have conflicting experimental demands
  - Recommendation: dedicated setups to these
    - Variable temperature
    - Short/long cooldown
    - Electronics
  - Iterate on qubit measurement setup:
    - Thermal, IR and B field isolation discussions with Rigetti, NIST etc







# Materials Characterization

Akshay Murthy

Lin Zhou

Michael Bedzyk

October 18, 2022

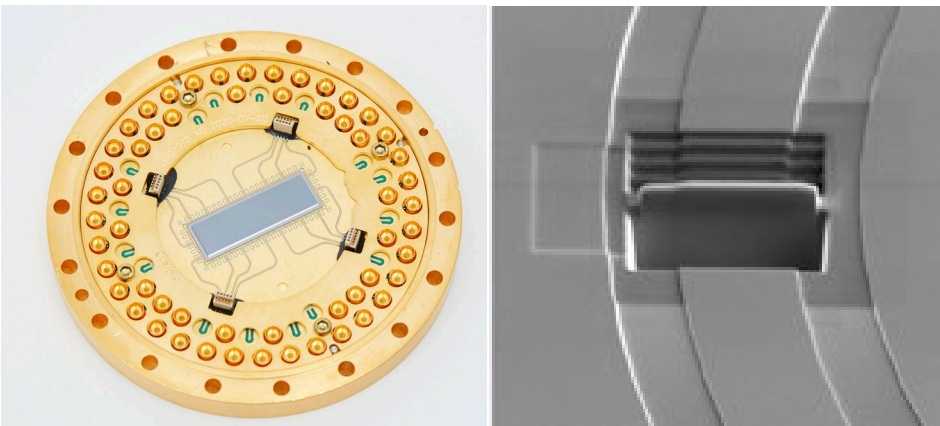
# Materials Characterization

		(3) Two Level Systems and Surface Passivation <i>Impacts: (4), (5)</i> <i>Drives: (1), (2)</i>	Identify theoretically and experimentally best techniques for comprehensive interface characterization and initial loss mitigation for TLSs							← Completed
			Several candidates for TLS based on detailed comparative structural studies of “bad” vs “good” transmons							← Completed
			Exploring niobium passivation techniques compatible with SRF cavities							
			Exploring niobium/aluminum oxide removal and passivation techniques compatible with 2D transmons <i>*Risk mitigation: by studying TLS reduction and surface passivation in both 2D and 3D structures, lessons learned can be transferred between groups</i>							
			Develop an atomic-level mechanistic understanding of TLSs							← In Progress

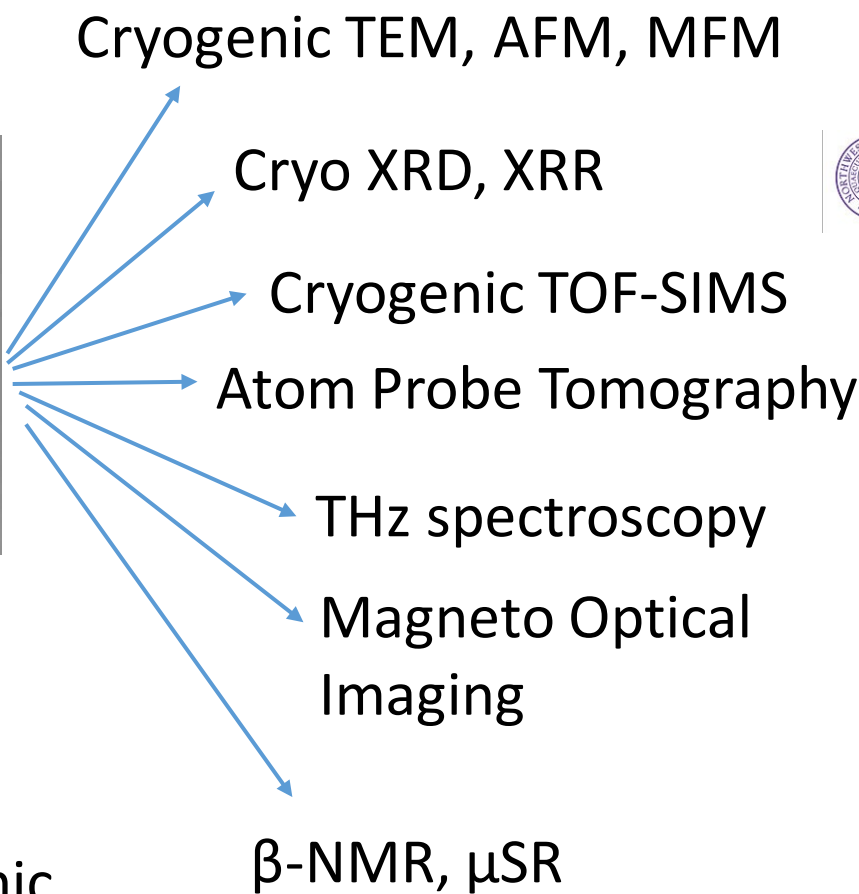
- **Goal:** Understand atomic and nanoscale sources of decoherence in superconducting qubits and sensors
- Allows for systematic improvement of coherence times in quantum devices

# How are we addressing this challenge?

Dissecting and studying fragments of characterized devices



- Leveraging DOE and SQMS academic partners user facilities capabilities to identify sources of decoherence





Northwestern University



Northwestern University Atomic and Nanoscale Characterization Experimental Center



AMES LABORATORY

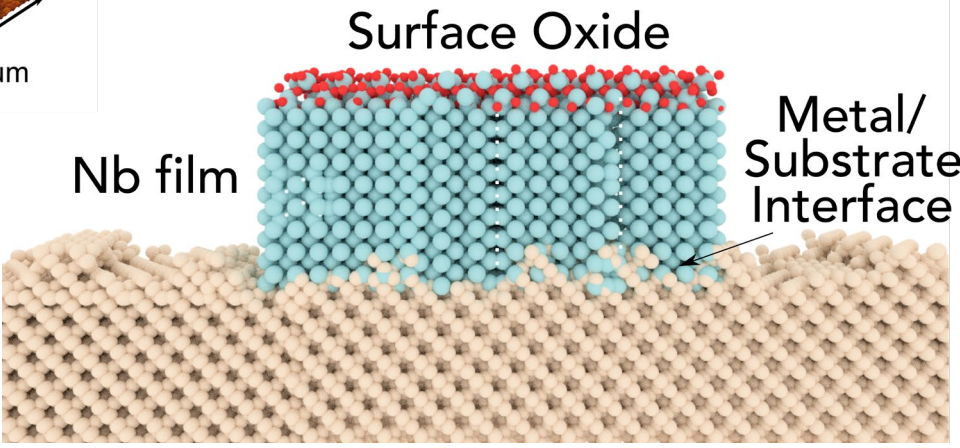
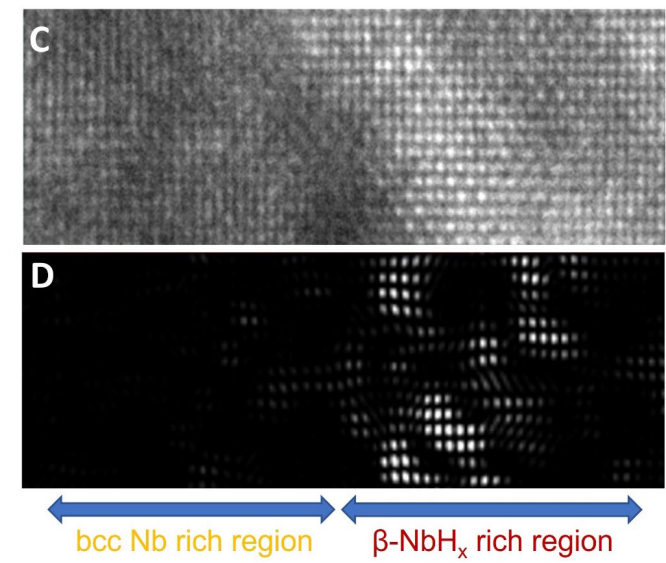
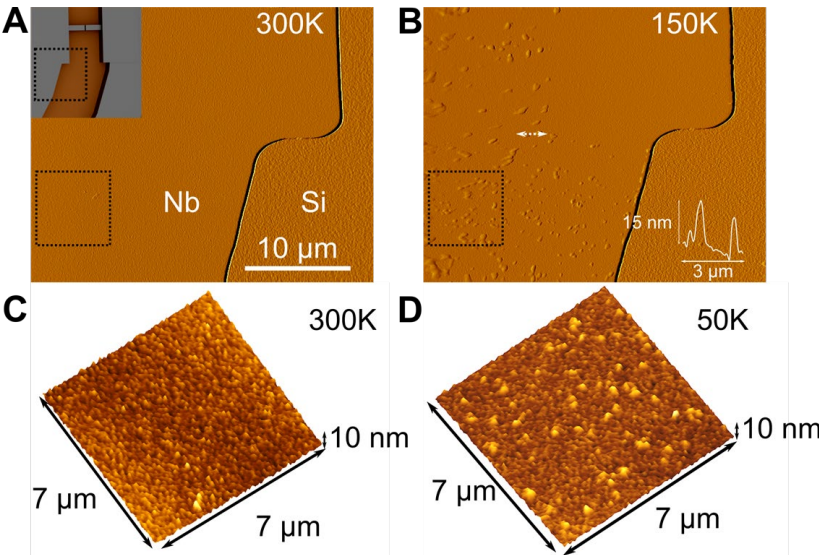


SIF SENSITIVE INSTRUMENT FACILITY



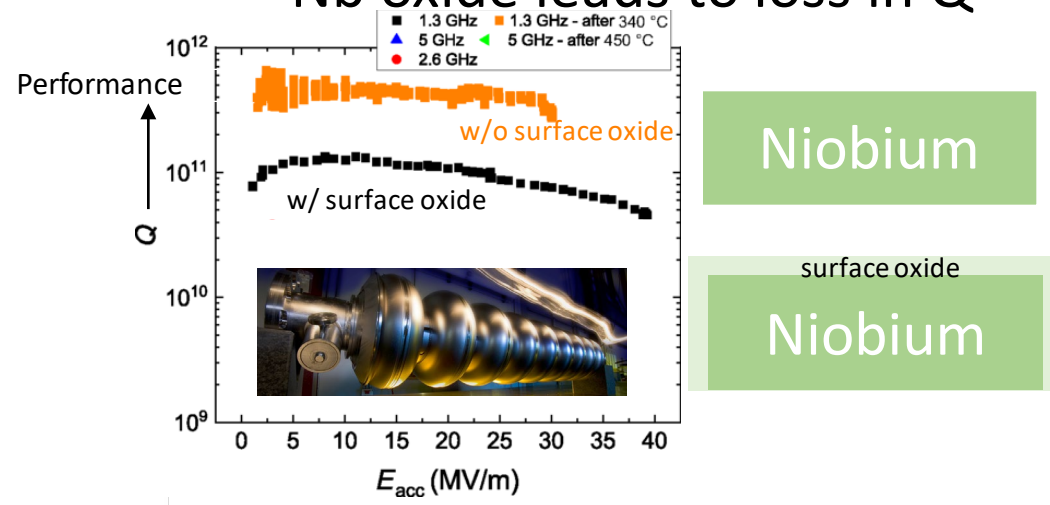


# Potential sources of decoherence

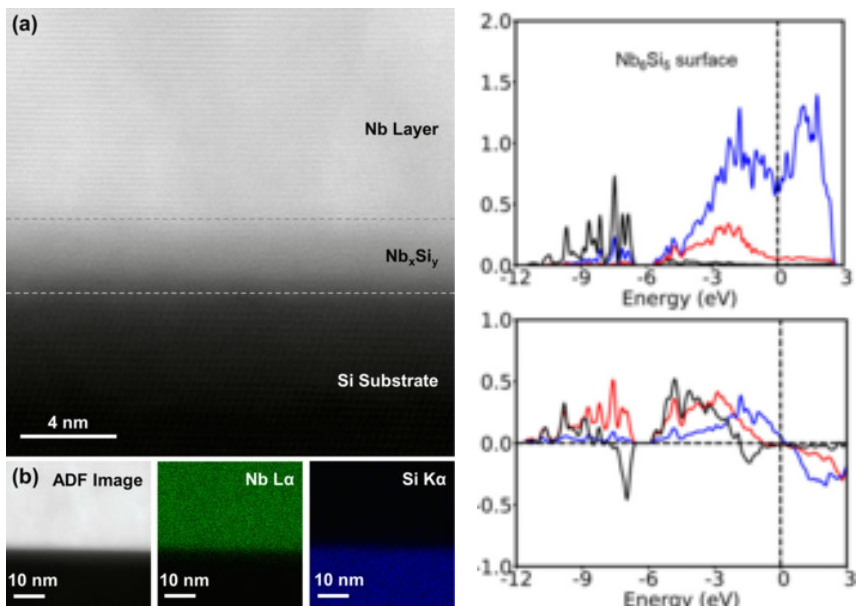


Nanohydrides form at cryogenic temperatures

## Nb oxide leads to loss in Q



Nb silicides may disrupt superconductivity



# Selected publications

- [1] Daniel Bafia, Anna Grassellino, Alexander Romanenko, “Probing the Role of Low Temperature Vacuum Baking on Photon Lifetimes in Superconducting Niobium 3-D Resonators”, preprint arXiv:2108.13352 (2022), submitted to PRAppl.
- [2] Akshay A. Murthy, Paul Masih Das, Stephanie M. Ribet, Cameron Kopas, Jaeyel Lee, Matthew J. Reagor, Lin Zhou, Matthew J. Kramer, Mark C. Hersam, Mattia Checchin, Anna Grassellino, Roberto dos Reis, Vinayak P. Dravid, Alexander Romanenko, “Developing a Chemical and Structural Understanding of the Surface Oxide in a Niobium Superconducting Qubit”, ACS Nano
- [3] Jin-Su Oh, Xiaotian Fang, Tae-Hoon Kim, Matt Lynn, Matt Kramer, Mehdi Zarea, James A. Sauls, A. Romanenko, S. Posen, A. Grassellino, Cameron J. Kopas, Mark Field, Jayss Marshall, Hilal Cansizoglu, Joshua Y. Mutus, Matthew Reagor, and Lin Zhou, Multi-modal electron microscopy study on decoherence sources and their stability in Nb based superconducting qubit. arXiv:2204.06041
- [4] Xiaotian Fang, Jin-Su Oh, Matt Kramer, A. Romanenko, A. Grassellino, John Zasadzinski, Lin Zhou, Materials Research Letter, 11, 108 (2023)
- [5] Mattia Checchin, Daniil Frolov, Andrei Lunin, Anna Grassellino and Alex Romanenko, “Measurement of the Low-Temperature Loss Tangent of High-resistivity Silicon Wafers with High-Q Superconducting Resonators”, preprint arXiv:2108.08894 (2021).
- [6] X. Lu, D. P. Goronzy, C. G. Torres-Castanedo, P. Masih Das, M. Kazemzadeh-Atoufi, A. McFadden, C. R. H. McRae, P. W. Voorhees, V. P. Dravid, M. J. Bedzyk, M.C. Hersam, and J. M. Rondinelli, “Stability, metallicity, and magnetism in niobium silicide nanofilms”, Physical Review Materials 6, 064402 (2022).
- [7] Jaeyel Lee, Zuhawn Sung, Akshay A. Murthy, Matthew Reagor, Anna Grassellino, and Alex Romanenko, “Discovery of Nb hydride precipitates in superconducting qubits”, preprint arXiv:2108.10385 (2021).
- [8]. R. Joshi, S. Ghimire, M. A. Tanatar, A. Datta, J.-S. Oh, L. Zhou, C. J. Kopas, J. Marshall, J. Y. Mutus, J. Slaughter, M. J. Kramer, J. A. Sauls, and R. Prozorov, “Quasiparticle Spectroscopy, Transport, and Magnetic Properties of Nb Films Used in Superconducting Transmon Qubits”, arXiv:2207.11616 (2022).
- [9] R. H. J. Kim, J. M. Park, S. Haeuser, C. Huang, D. Cheng, T. Koschny, J. Oh, C. Kopas, H. Cansizoglu, K. Yadavalli, J. Mutus, L. Zhou, L. Luo, M. Kramer, J. Wang. Visualizing heterogeneous dipole fields by terahertz light coupling in individual nano-junctions used in transmon qubits. [arXiv:2207.05960] (2022).

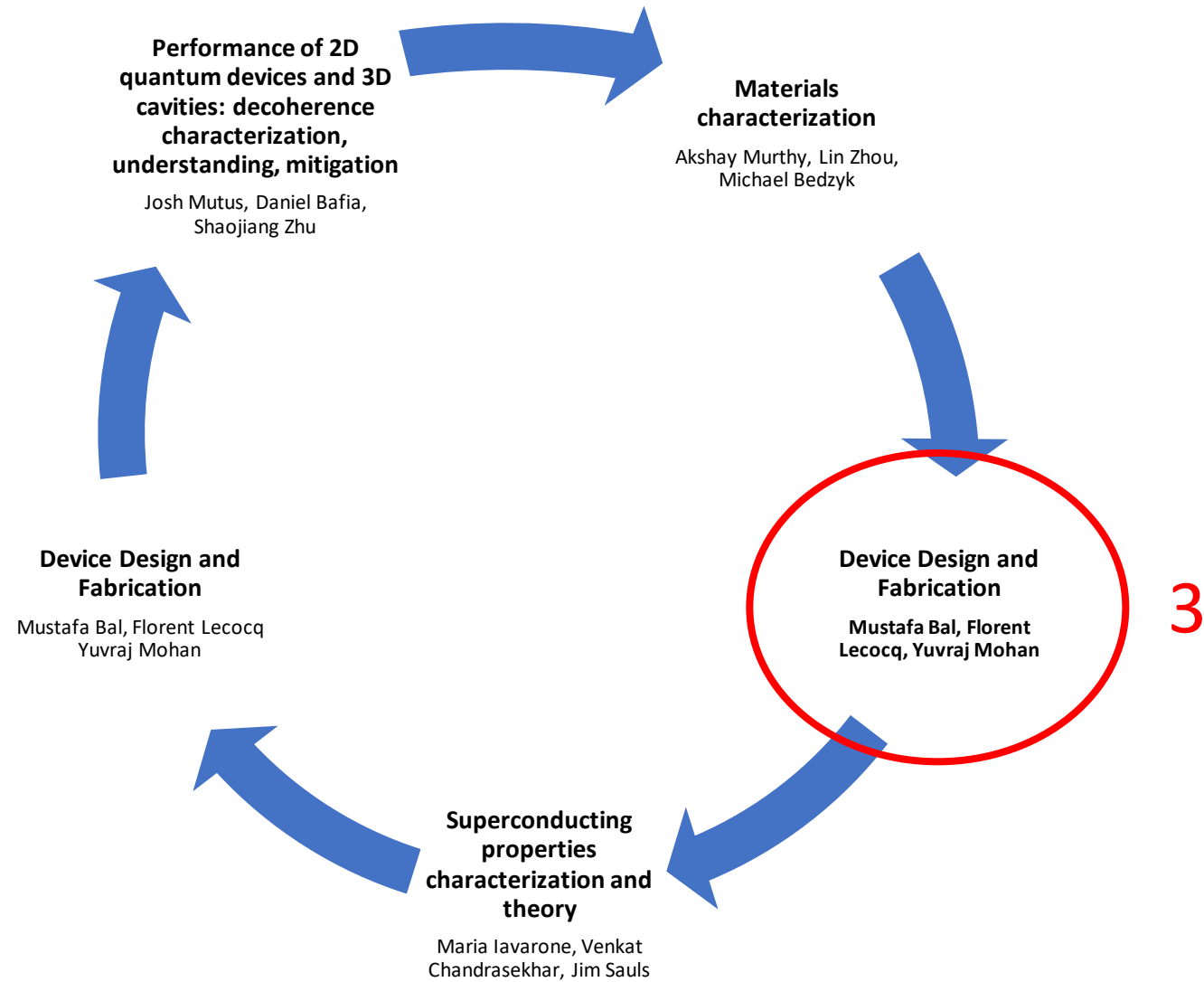
## Potential sources of decoherence

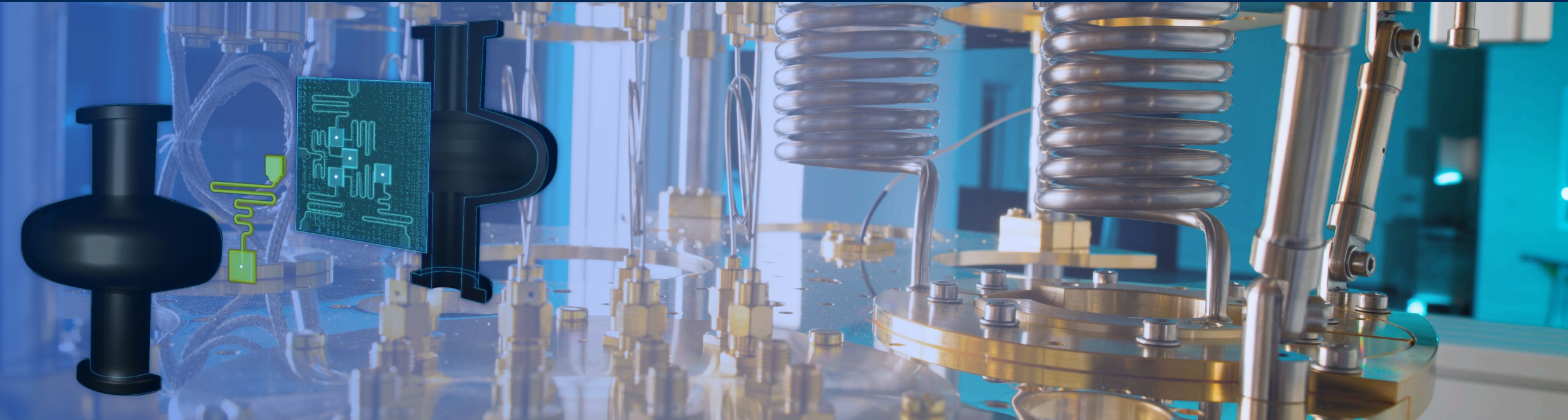
- Partial dissolution of surface oxide leads to an increase in two-level system (TLS) induced losses through oxygen vacancy formation in Nb [1]
  - Relationship between local disorder in Nb<sub>2</sub>O<sub>5</sub> and oxygen sub-stoichiometry may play a role in decoherence in superconducting qubit devices [2].
  - Temperature cycling leads to the formation of FCC Nb nanocrystals in the surface oxide [3];
  - Nitrogen doping introduces surface strain/stress and reduced surface oxide thickness [4];
- First direct measurement of the low-temperature loss tangent of high-resistivity silicon with a high Q-factor superconducting resonator [5]. This platform enables the characterization of the microwave loss associated with various dielectrics and substrates. Results were a clear demonstration of the impact of silicon on decoherence of qubits.
  - Detailed characterization and understanding of niobium silicide interfacial layers formed through sputter deposition of Nb films on silicon substrates indicate that Nb-Si heterointerfaces in 2D transmon structures are not atomically sharp [3, 6]
- Formation of niobium hydrides throughout the Nb film at cryogenic operating temperatures can potentially serve as a TLS mechanism and/or introduce loss [7,8]
  - Terahertz nano-imaging reveals asymmetry in charge scattering across the junction due broken boundaries from two angled Al evaporation deposition procedures. [9]



## What still needs to be done to reach center-wide deliverable? What are the long term goals?

- Two-level systems and surface passivation
  - Detailed comparative structural studies on “good” and “bad” transmons
  - Atomic level mechanistic understanding of TLS
- Continue to evaluate tested qubit devices with state-of-the-art methods
- Continued integration between materials synthesis and materials characterization
- What new techniques make sense?
  - *In situ* (cryogenics, time-resolved, microwave stimulation)
- Build decoherence model based on microwave measurements
- Center-wide review paper on origin of TLS in 2D transmon
- Should be a comprehensive paper pulling together the fabrication, testing, characterization of key defects (good/bad regions) and supporting theory





# Device Design and Fabrication

Florent Lecocq (NIST)

Mustafa Bal (FNAL)

Yuvraj Mohan (Rigetti)

**NIST**  
National Institute of  
Standards and Technology  
U.S. Department of Commerce

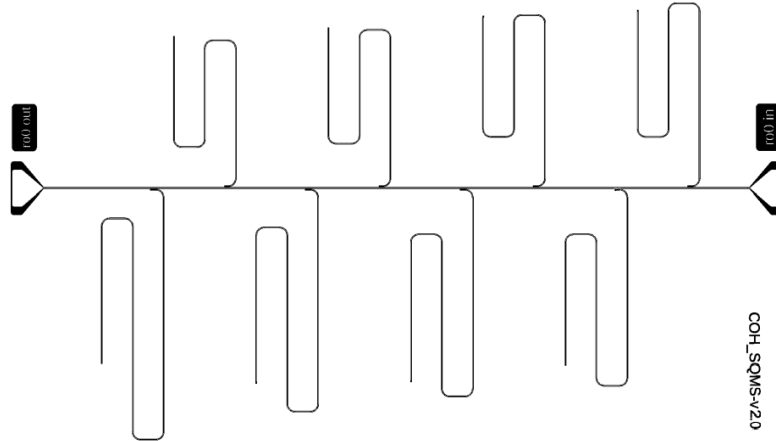
**rigetti**

10/18/2022

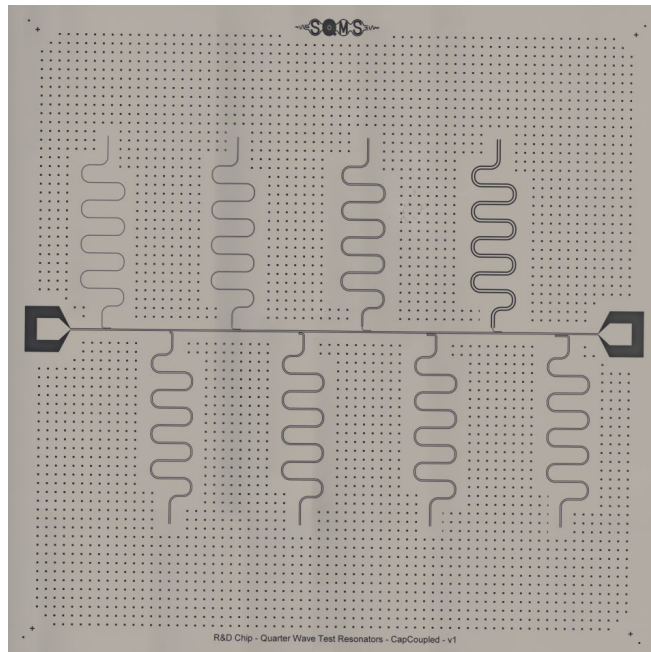
Northwestern

**AMES**  
NATIONAL LABORATORY  
Creating Materials & Energy Solutions

# SQMS R&D Resonator Design – v1



[arXiv:2204.07202](https://arxiv.org/abs/2204.07202)



## Scientific Achievement

Standardized resonator chips have been designed to be used for encapsulation studies.

## Significance and Impact

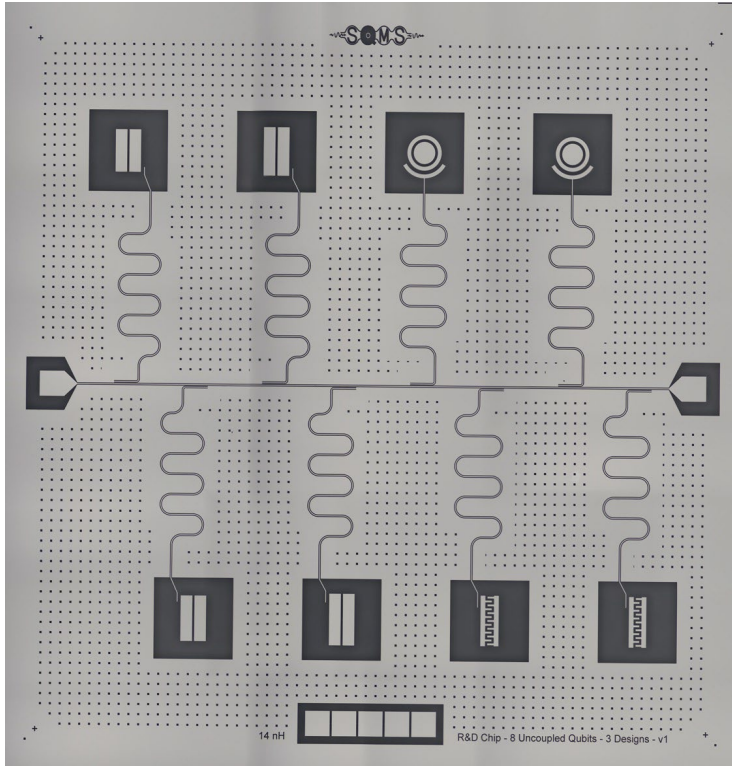
The same resonator chip design will be used by all fab teams across the SQMS Center. This will enable a direct comparison of results and converge on materials and processes that yield better qubit coherence.

## Details

- 8 resonators
- Readout resonators frequency  $\sim 4 - 8$  GHz
- Frequency multiplexing on single feedline
- Qc between 200k and 10M



# SQMS R&D Qubit Design – v1



Microscope image of a SQMS R&D Chip

## Scientific Achievement

A standardized qubit chip has been designed to be used for encapsulation studies.

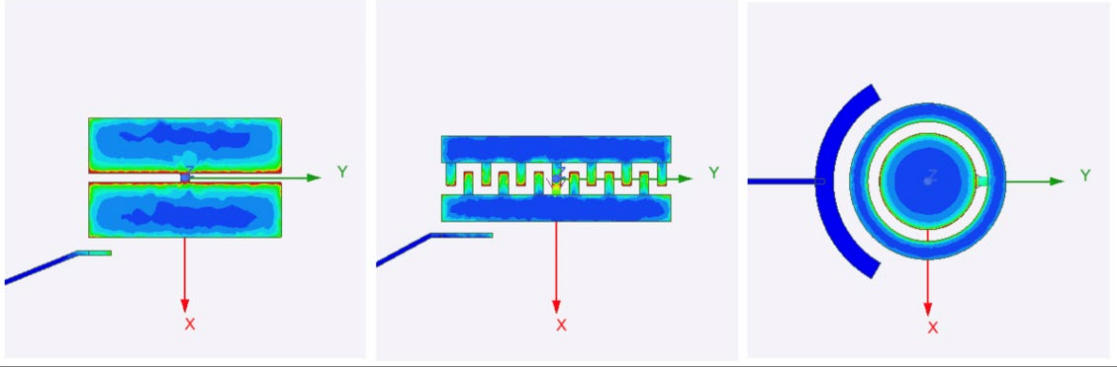
## Significance and Impact

The same qubit chip design will be used by all fab teams across the SQMS Center. This will enable a direct comparison of results and converge on materials and processes that yield better qubit coherence.

## Details

- 8 fixed frequency uncoupled transmons  $\sim 4 - 5$  GHz
  - 4 w/ double capacitive pads (for statistics)
  - 2 w/ interdigitated capacitive pads (most sensitive)
  - 2 w/ concentric capacitive pads (most insensitive)
- Anharmonicity  $\sim 220$  MHz
- Readout resonators  $\sim 6 - 8$  GHz
- Frequency multiplexing on single feedline

# SQMS R&D Qubit Design – v1



E-field Distribution of different transmon geometries

## Scientific Achievement

A standardized qubit chip has been designed to be used for encapsulation studies.

## Significance and Impact

The same qubit chip design will be used by all fab teams across the SQMS Center. This will enable a direct comparison of results and converge on materials and processes that yield better qubit coherence.

Double Pad Transmon

	$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
0	7596.0	5054.0	0.42	308.0	88.0	0.8	10000	0.0009
1	7515.0	4958.0	0.40	296.0	89.0	0.8	10000	0.0009
2	7428.0	4916.0	0.42	290.0	90.0	0.7	10000	0.0009
3	7348.0	4861.0	0.43	284.0	91.0	0.7	10000	0.0010

IDC Transmon

	$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
4	7232.0	4465.0	0.35	235.0	102.0	0.7	10000	0.0010
5	7141.0	4399.0	0.36	228.0	105.0	0.7	10000	0.0010

Concentric Transmon

	$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
6	6748.0	4340.0	0.33	223.0	88.0	0.7	10000	0.0009
7	6626.0	4320.0	0.37	221.0	90.0	0.7	10000	0.0010

$L_j=14\text{nH}$  & Sapphire Substrate ( $\epsilon_s = 10.0$ )

$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
7716.0	5122.0	0.39	266.0	94.0	0.8	10000	0.0010
7551.0	4971.0	0.40	249.0	98.0	0.8	10000	0.0011
7382.0	4813.0	0.39	233.0	100.0	0.7	10000	0.0011
7214.0	4690.0	0.40	220.0	102.0	0.7	10000	0.0012

$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
7002.0	4545.0	0.39	205.0	102.0	0.7	10000	0.0012
6835.0	4462.0	0.40	197.0	103.0	0.7	10000	0.0013

$f_r$	$f_{01}$	$\chi$	$\alpha$	$g$	$\kappa$	$Q_c$	$\gamma$
6431.0	4332.0	0.31	187.0	81.0	0.6	10000	0.0010
6268.0	4283.0	0.39	182.0	87.0	0.6	10000	0.0012

$L_j=12\text{nH}$  & Si Substrate ( $\epsilon_s = 11.9$ )



# SQMS Nanofabrication Taskforce

- Conduct coordinated studies to improve coherence in quantum devices across the various SQMS foundries
- Share technical knowledge to implement novel fabrication processes
- Make recommendations on fabrication processes and materials for improved quantum device performance
- Make recommendations on next generation fabrication tools for improved quantum device performance
- Guided by materials studies, explore novel device geometries for improved quantum device performance
- Train students and postdocs.



Leader: Mustafa Bal (FNAL)



# Encapsulation Study of Nb for Improved Qubit Coherence

Substrates	Superconducting Thin Films	Encapsulation	FNAL/PNF	NIST	Rigetti	Northwestern (limited to film deposition and passivation, qubits to be made at PNF)
1 – Sapphire (C-plane, R-plane)  *FNAL, NIST to prioritize sapphire  2 – Silicon (of different resistivity and orientation)  ** Rigetti will fab on silicon, NU to focus also on Si 111	Nb	Native Oxide	X Baseline	X Baseline	X Baseline	X Baseline (Si 100, Si 111, Sa)
		Al	X		X	
		Ta	X	X	X	
		Re	X			
		Au	X	X		
		TiN	X	X		X
		NbN				
		Pt				X
		Semiconductor (Si, Ge..)				X

Work details of Nb Encapsulation Study

## Scientific Achievement

A coordinated study is launched across SQMS Center to encapsulate Nb surface to prohibit the formation of NbOx.

## Significance and Impact

In the first 2 years of center wide research, NbOx is singled out as a major source of qubit decoherence. Replacing NbOx with another material could potentially reduce the loss and hence enhance qubit coherence time.

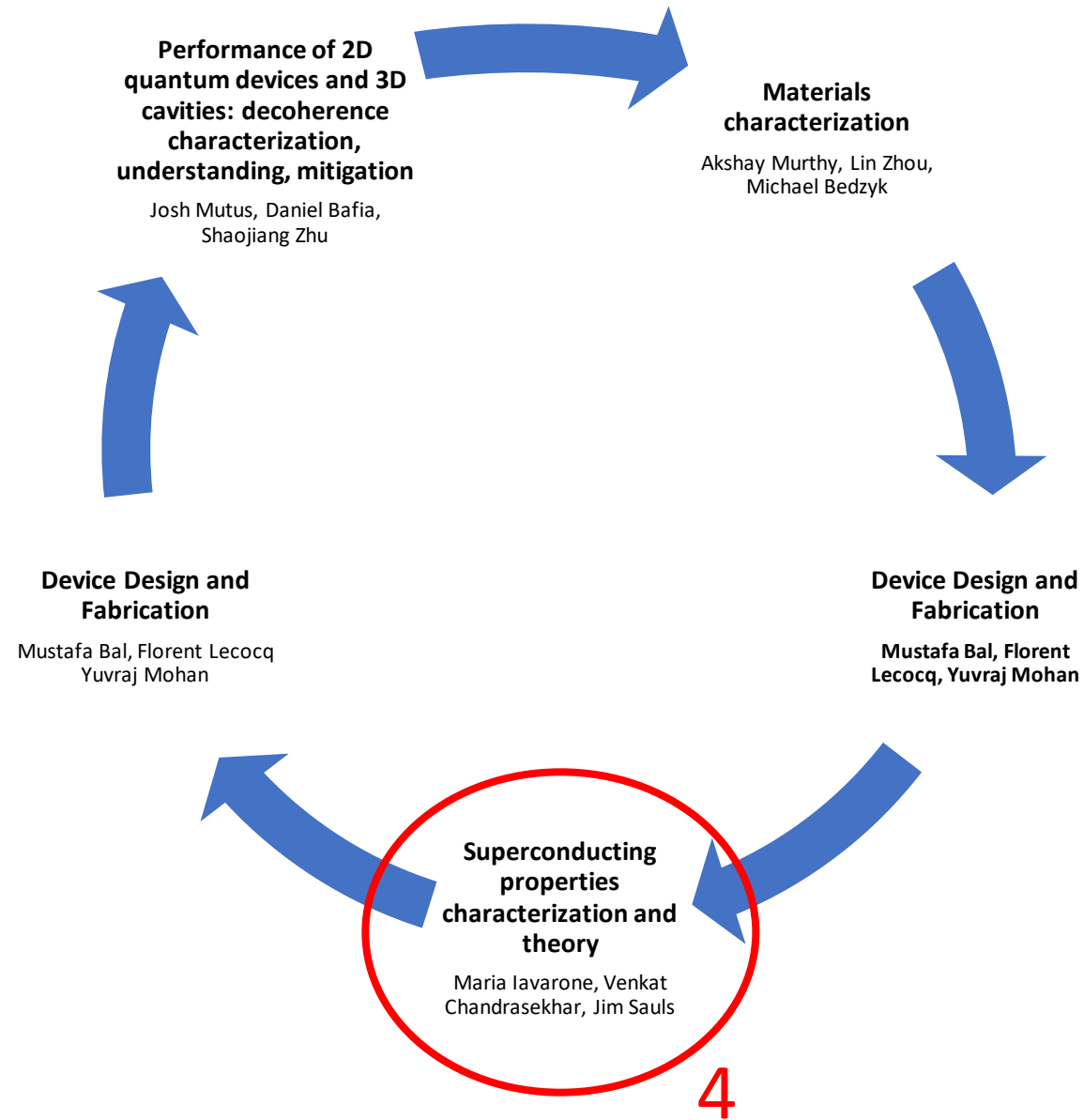
## Details

5 to 10 nm of encapsulation layer will be deposited on Nb surface. Potential encapsulation materials include Al, Ta, and Au, to name a few. FNAL, NIST, Rigetti and NU will participate in this study as shown in the table.

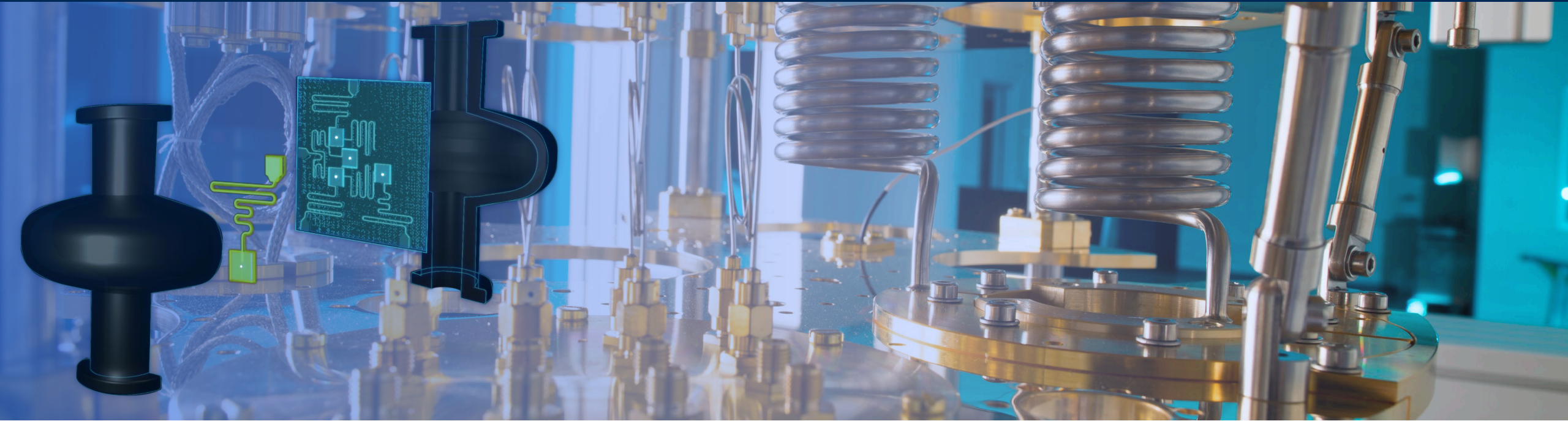
# What still needs to be done?

Focus Area	Major Activity	Deliverables and Benchmarks	Center Year				
			1	2	3	4	5
	(3) Two Level Systems and Surface Passivation <i>Impacts: (4), (5)</i> <i>Drives: (1), (2)</i>	Identify theoretically and experimentally best techniques for comprehensive interface characterization and initial loss mitigation for TLSs					
		Several candidates for TLS based on detailed comparative structural studies of “bad” vs “good” transmons					
		Exploring niobium passivation techniques compatible with SRF cavities					
		Exploring niobium/aluminum oxide removal and passivation techniques compatible with 2D transmons <i>*Risk mitigation: by studying TLS reduction and surface passivation in both 2D and 3D structures, lessons learned can be transferred between groups</i>					
		Develop an atomic-level mechanistic understanding of TLSs					
	(4) Transmon Coherence Time Milestones <i>Impacts: (6), (7), (10), (13), (14)</i> <i>Drives: (1), (2), (3)</i>	transmons to achieve maximum individual coherence times > 1 ms					
		Delineate specifications for bulk substrate materials to ensure coherence of transmon > 1 ms with spread < 20%					
		Modify manufacturing procedures and/or post-manufacturing treatments of 2D superconducting transmons to achieve coherence times > 1 ms with less than 20% spread					

- Materials and fabrication processes need to be developed to realize various encapsulations on Nb.
- Transmon qubits with encapsulations need to be screened to converge on the materials and processes for improved coherence
- A long road ahead: systematic testing, large parameter space!







# Superconducting Properties Characterization and Theory

Maria Iavarone

Venkat Chandrasekhar

Jim Sauls



10/18/2022





## What appendix 13 activity and/or WBS deliverable do these activities address?

### Materials for 2D and 3D Quantum Devices



#### Advanced Materials Studies

- Spectroscopic and superconducting properties investigations of Nb and Al in the full quantum regime (e.g., penetration depth, STM, STS)



#### Two Level Systems and Surface Passivation

- Identify theoretically and experimentally best techniques for comprehensive interface characterization and initial loss mitigation for TLSs
- Exploring Nb passivation techniques compatible with SRF cavities
- Explore Niobium/Aluminum oxide removal and passivation technique compatible with transmon
- Develop an atomistic-level mechanism understanding of TLS

2D

## How are we addressing this challenge?

- ❑ Theory/ First Principle Calculations
- ❑ Transport Measurements
- ❑ Tunneling experiments using point contact and STM
- ❑ Magneto optical imaging
- ❑ THz/GHz conductivity spectroscopy and imaging

## List of the activities (1)

- **Revealing Microscopic Properties of Nb via Transport:** Phase boundary studies have helped to determine changes to the superconducting coherence length related to Nb film grain structure and epitaxy
- **Quasiparticle spectroscopy via London penetration depth:** Precision measurements of London penetration depth reveal the superconducting gap structure and sub-gap excitation spectrum.
- **Scanning Point Contact Tunneling of SRF Cavity Nb:** Large Area ( $200 \times 300 \mu\text{m}^2$ ) maps of superconducting  $\Delta$  and Nb Oxide Properties (Barrier Height, Thickness, Magnetism). (Surface oxide properties depends on Nb Processing)
- **Gap and Scattering Parameter Maps:** Gap maps show gap variations of about 20% over an area of 200 nm (possible QPs trapping and SC weakening)
- **Near-surfaces magnetic impurities in annealed Nb films:** Experimental proof of the presence of localized magnetic impurities near-surface of annealed Nb films at 400 °C.

## List of activities (2)

- **THz spectroscopy of Nb superconductivity and quasi-particle scattering:** THz conductivity of Nb film was studied with THz and pump probe spectroscopy and revealed a quasi-particle scattering peak  $\sim \Delta_{sc}$ .
- **Effects of disorder on anisotropic superconductivity in Nb:** Experimental proof of an anisotropic superconducting state of niobium in quantitative agreement with theoretical predictions.
- **Microwave characterization of disorder in superconducting resonators:** Developed first principles theory for the effects of disorder on Nb-based superconducting resonators that provides precision microwave characterization of the effects of disorder on the resonance frequency
- **Effects of disorder on anisotropic superconductivity in Nb:** Experimental proof of an anisotropic superconducting state of niobium. **Nb is an anisotropic superconductor in which non-magnetic disorder is pair-breaking, generating sub-gap quasiparticle states**
- **Pure Nb is an intrinsic type-I superconductor**

## Conclusions (from my point of view)

- Studying phenomenological solutions to tackle effects of niobium oxide through encapsulation
- More tests to understand/measure Si and Al<sub>2</sub>O<sub>3</sub> loss
- Need to broaden the horizon to other elements (Al JJ , QPs?)
- Need of more measurements on 2D devices
- A lot of work on material characterisation still need to be linked to the real case



## BACKUP SLIDES

# Key Areas and Unknowns

- Known sources of decoherence & eliminating those sources
  - $T_1$  is a convoluted metric, we need to develop protocols and theory to better understand specific loss mechanisms.
    - There are many factors from design, processing, and materials
  - We have yet to clearly identify specific sources of decoherence.
    - Other measurements such QP generation, superconducting gap, upper critical field, and London penetration depth, etc. may be better means of better characterizing sources of decoherence.
    - Can we better use theory to identify specific measurements or test ideas about sources of decoherence, especially in the temperature and frequency domain.

# Niobium suboxides as a source of TLS Losses

D. Bafia, A. Grassellino, and A. Romanenko [arXiv:2108.13352](https://arxiv.org/abs/2108.13352)

## Scientific Achievement

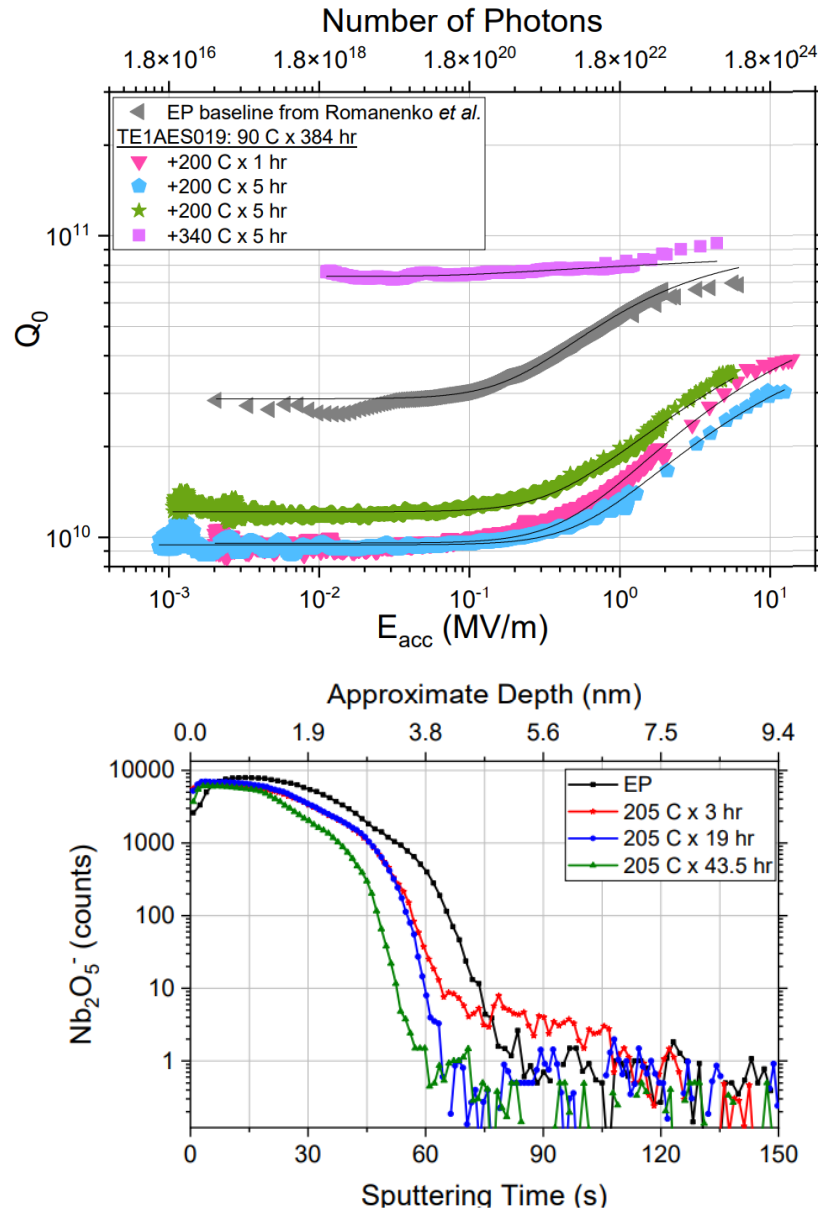
Found evidence which suggests that magnetic niobium suboxides (non-stoichiometric  $\text{Nb}_2\text{O}_5$ ,  $\text{NbO}$ ,  $\text{NbO}_2$ ) drive TLS losses in Nb cavities. Also showed the non-role of diffused oxygen in the low field performance of cavities.

## Significance and Impact

These results provide insights on the source of TLS-driven losses in niobium oxides and further motivate studies into encapsulation methods. Moreover, these findings suggest that partial oxide dissolution is particularly detrimental to qubit and cavity performance and must be avoided during fab.

## Details

- 2 cavities were subjected to sequential rounds of *in situ* vacuum baking to gradually dissolve the oxide and tested at 2 K.
- Recreating the vacuum baking treatment *in situ* in TOF-SIMS on a cavity cutout confirm partial oxide dissolution and growth of suboxides.
- Non-monotonic dependence of low field  $Q_0$  due to interplay of magnetic suboxide generation and oxide thickness reduction.



# Characterization of Nb films with varying RRR values at low temperatures

B. Abdisatarov, G. Ereemeev, H. E. Elsayed-Ali, J. Lee, A. Lunin, C. P. A. Carlos and S. Leith, G. J. Rosaz, A. Grassellino, A. Romanenko

## Scientific Achievement

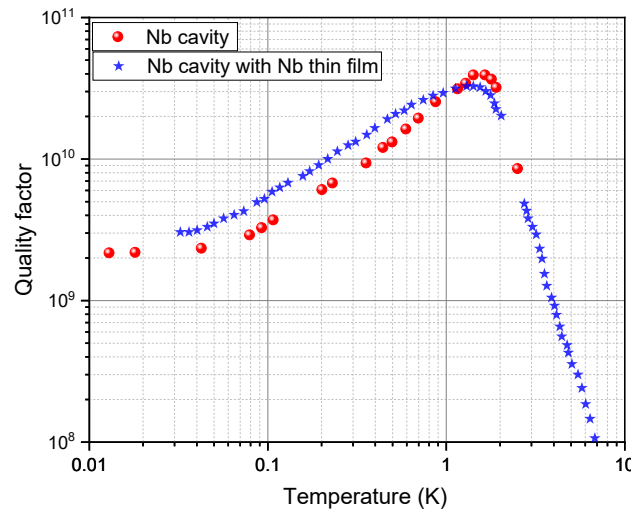
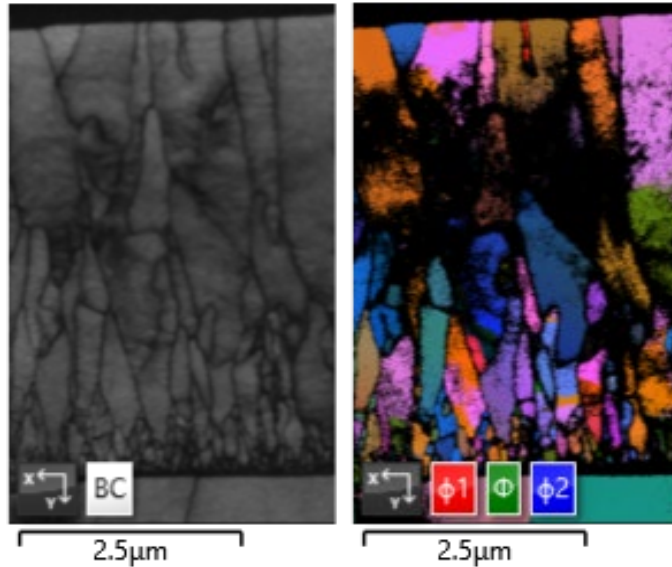
Nb film, deposited onto 1.3 GHz elliptical niobium cavity by HiPIMS technique at CERN, is processed with different treatments to understand the contribution of different loss mechanisms. The first results show that niobium film performance is comparable that of the bulk niobium cavities at low temperatures.

## Significance and Impact

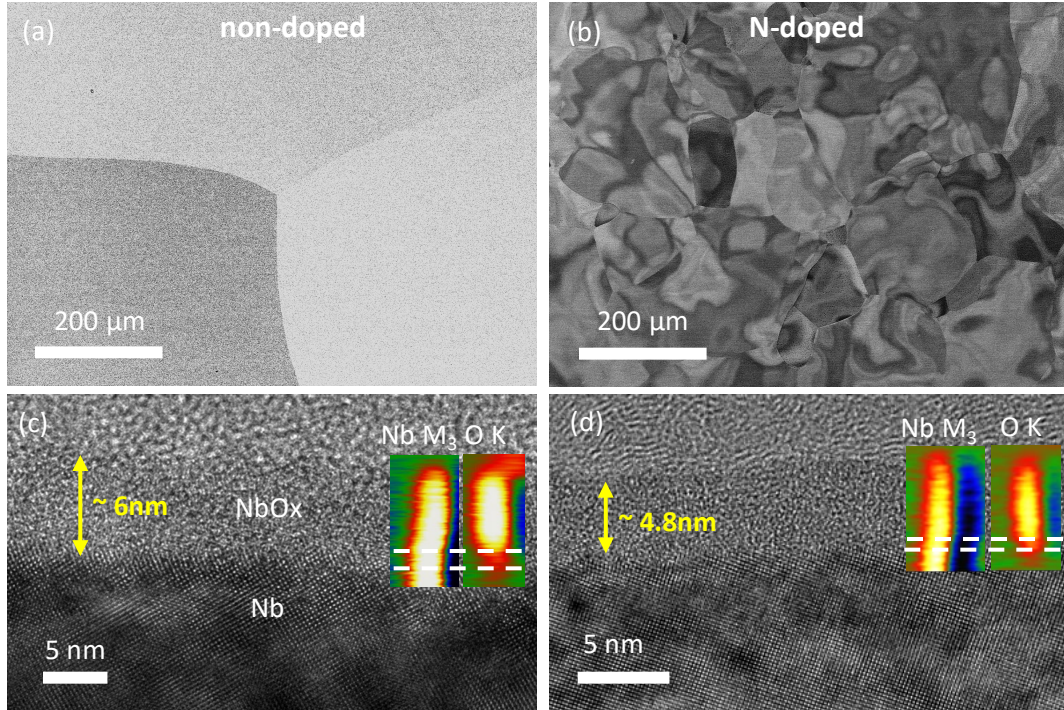
The results set apart different loss mechanisms in niobium films and points to the loss mechanism extrinsic to metallic niobium as the dominant source of microwave losses.

## Details

- Coated niobium film with HiPIMS techniques onto 1.3 GHz cavity in collaboration with CERN and Old Dominion University
- Measured the cavity with niobium film in low microwave fields down to 40 mK
- Estimated niobium film RRR of about  $\sim 20$ , which is significantly below  $RRR \sim 300$  for bulk niobium cavities
- Niobium film cavity performance is comparable to that of a bulk niobium cavity
- First results show that resistance of the film drops significantly after mid-T bake



# Nitrogen doping may alter stress state at the Nb/air interface in cavities



**Backscattered scanning electron microscopy** images of undoped (a) and N-doped (b) cavity samples. The contrast variation in the grains of the N-doped sample is caused by stress/strain close to the Nb/air interface.

**High-resolution transmission electron microscopy** image taken along [001] ZA of the undoped (c) and N-doped (d) cavity samples. The color insets are the first derivative of the electron-energy-loss spectroscopy line scan of the Nb-M<sub>3</sub> and O-K edges.

Xiaotian Fang, Jin-Su Oh, Matt Kramer, A. Romanenko, A. Grassellino, John Zasadzinski, Lin Zhou, *Materials Research Letter*, 11, 108 (2023)

<https://doi.org/10.1080/21663831.2022.2126737>

## Scientific Achievement

Nitrogen doping may alter stress state at the Nb/air interface, which impedes the oxygen and hydrogen atoms' diffusion and reduces surface oxide thickness.

## Significance and Impact

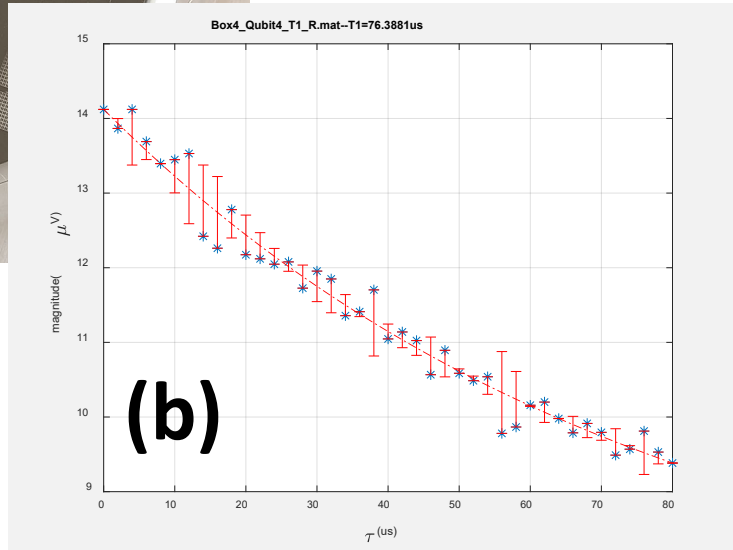
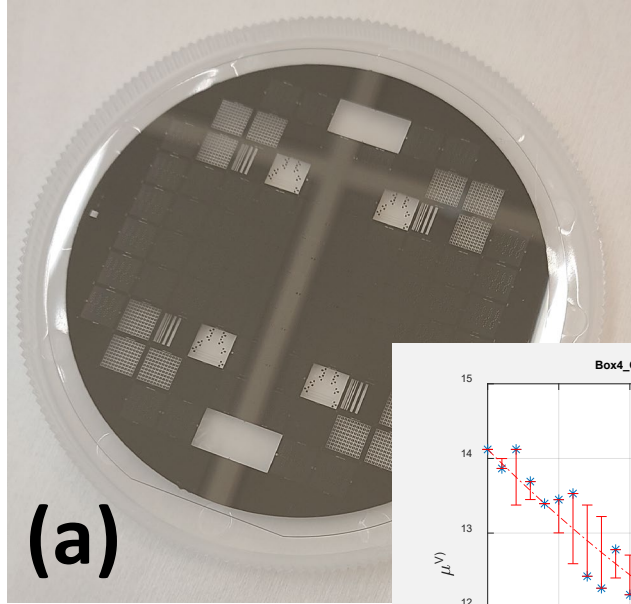
Established a mechanistic understanding of the role of dopants in Superconducting Radio Frequency Cavity fabrication which significantly increased their Q factor.

## Research Details

- Aberration-corrected (scanning) transmission electron microscopy were used to study the Nb/air interface.
- {100} and {110} Nb facets are observed at the Nb/NbO<sub>x</sub> interface.
- There is a valence state transition of Nb in the NbO<sub>x</sub> layer across the NbO<sub>x</sub>/Nb interface for both samples.
- Nitrogen atoms may diffuse into the octahedral interstitial sites of the Nb lattice causing high compressive stress/strain near the surface.
- The N atoms and compressive stress/strain impede the diffusion of oxygen atoms resulting in ~20% thickness reduction of the oxidation layer in the N-doped sample compared with the non-doped sample.



# Increased Nanofabrication Capability under SQMS Center



**First devices fabricated at PNF: (a) Photograph of processed 4" sapphire substrate. (b) T1 relaxation time of 1<sup>st</sup> batch of transmon qubit.**

## Scientific Achievement

Fermilab team started fabricating superconducting quantum devices at Pritzker Nanofabrication Facility (PNF) at University of Chicago.

## Significance and Impact

The addition of PNF to NIST & Rigetti foundries increased the wafer processing throughput more than twofold. The increased capacity will speed up SQMS Center in reaching its milestones.

## Details

Processes and capability is developed to fabricate superconducting quantum devices at PNF. Fermilab team successfully fabricated transmon qubits with long coherence time. The Nb encapsulation studies is expected to yield even longer coherence.

## What still needs to be done by the time of the technical review?

- In progress activities:
  - Nano-bridge measurements to study quasiparticle thermalization in Nb and Al
  - Nb single crystal measurements to study gap anisotropy. Integrated effort between theory and experiment.

