The Role of Nitrogen and Other Impurities in SRF Cavity Performance

Daniel Bafia

SRF 2023

June 27th, 2023

FERMILAB-SLIDES-23-135-SQMS-TD

The Versatile Bulk Nb Superconducting Radio-Frequency Cavity

Particle Acceleration

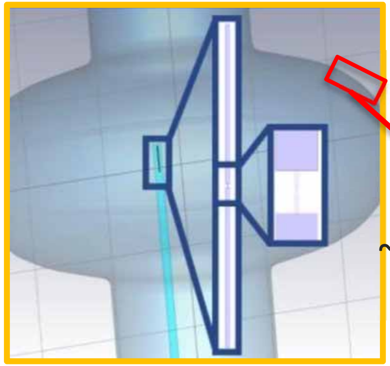
[redacted]

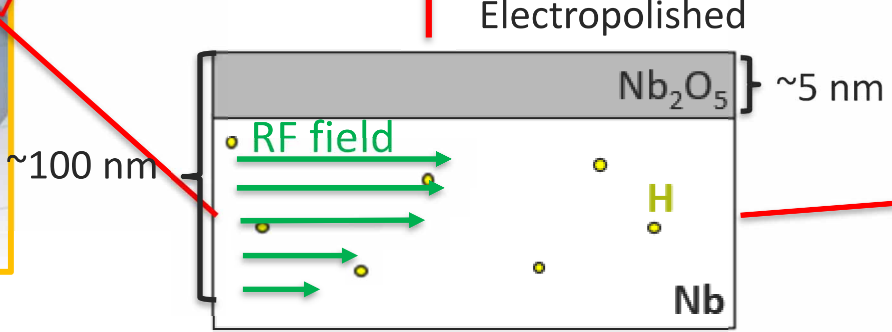
Sensitive Detectors

See talk by B. Giaccone, Thursday

Quantum Computing

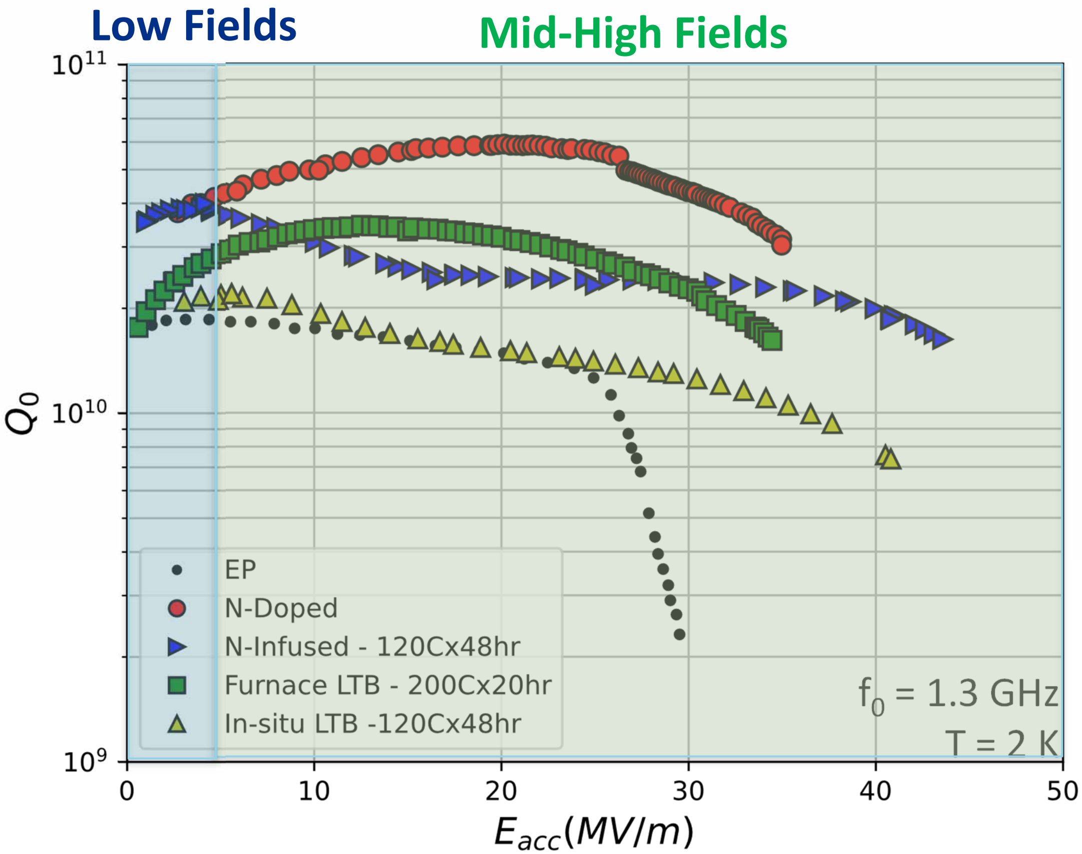
See talk by T. Roy, Friday



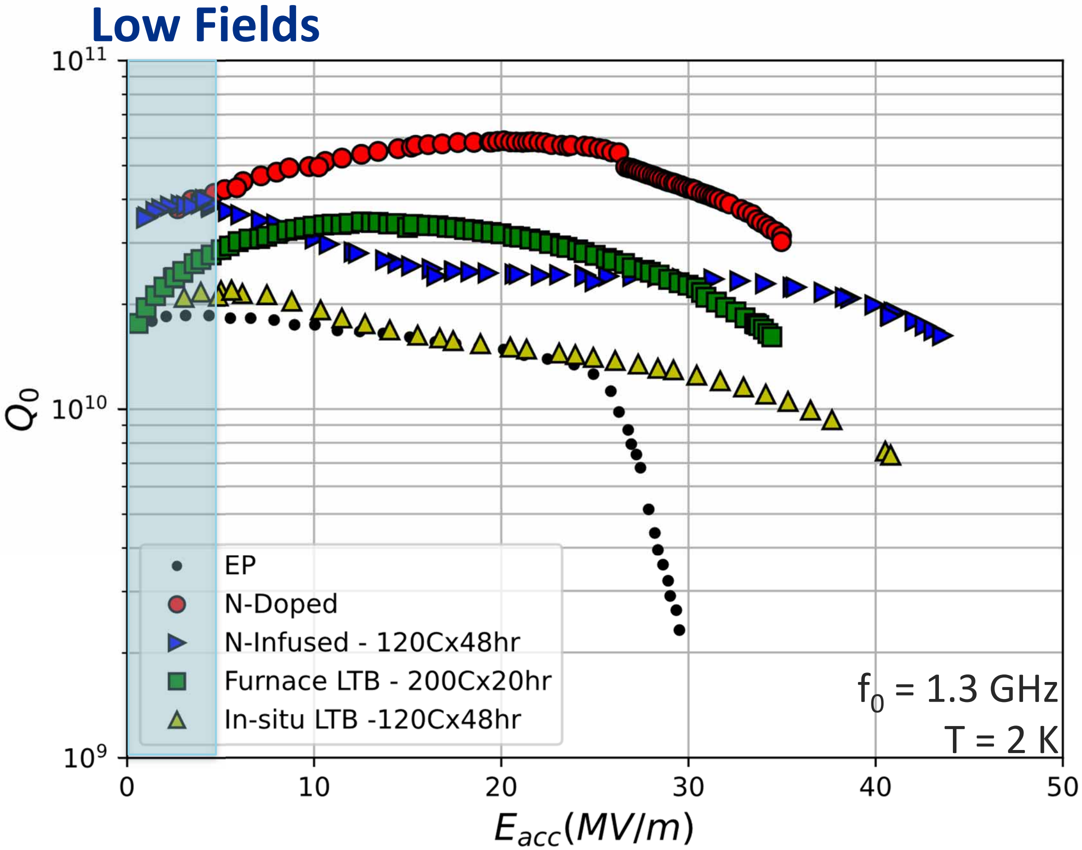


Recent Q advancements have enabled applications of SRF cavities to new fields!

Tailoring Cavity Performance via Surface Processing Techniques

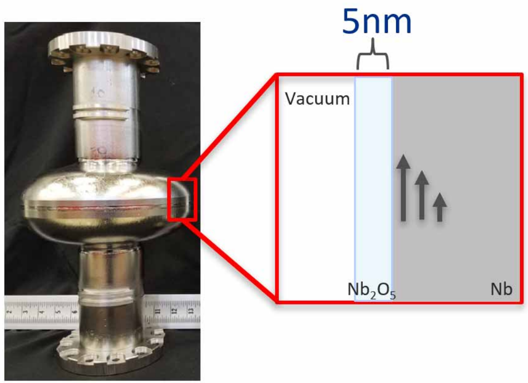


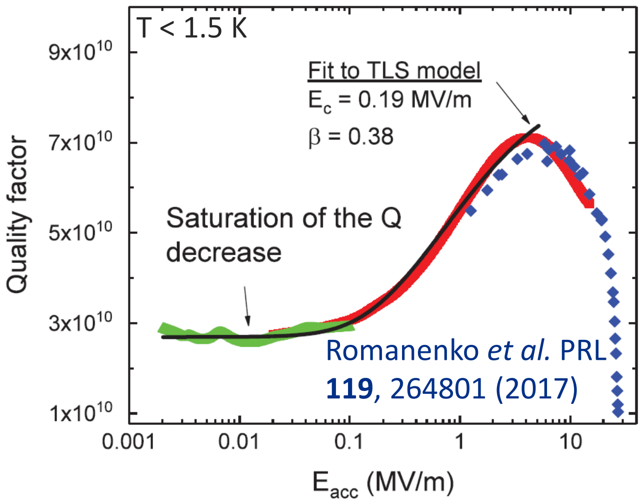
Tailoring Cavity Performance via Surface Processing Techniques

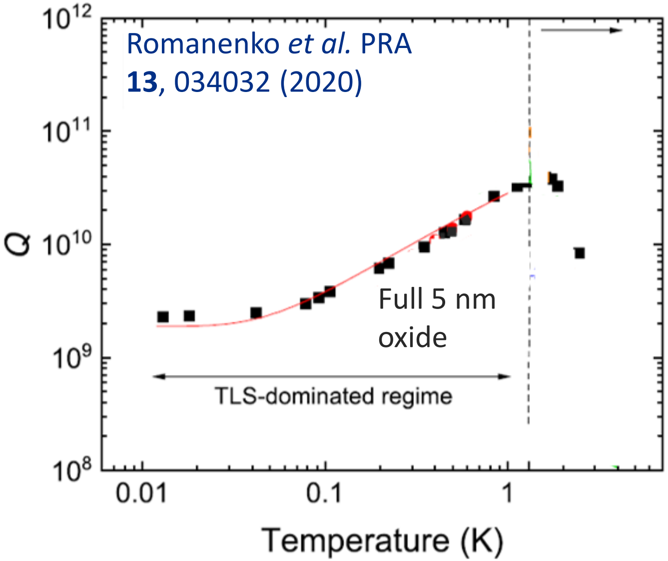


Identifying Sources of Loss in the Low Field and Quantum Regime

- FNAL demonstrated that low field Q slope is caused by amorphous native Nb oxide – host “Two-Level Systems (TLS) losses”



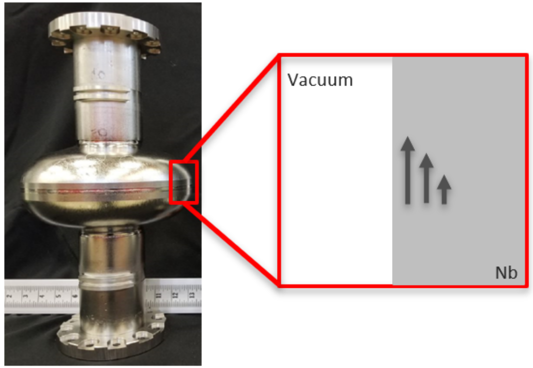




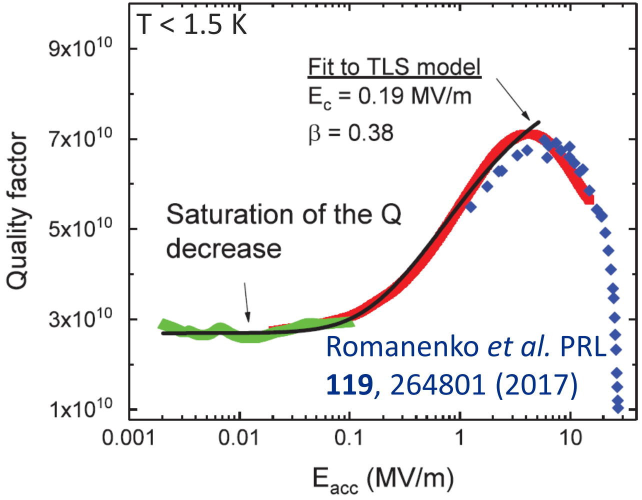
Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

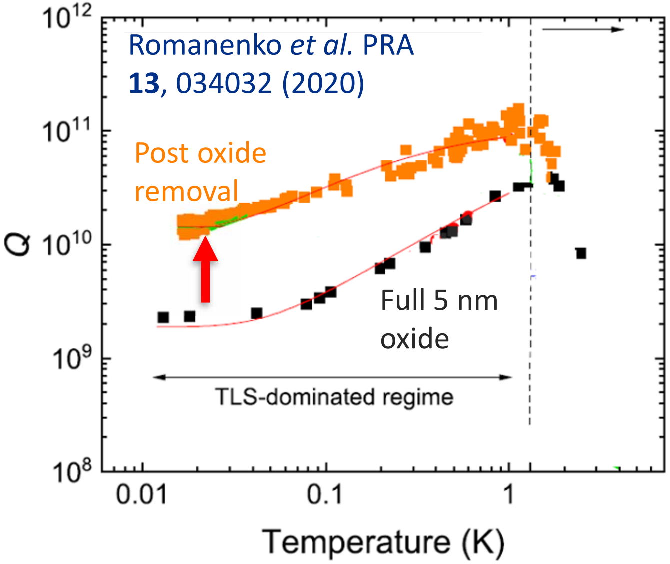
Identifying Sources of Loss in the Low Field and Quantum Regime

- FNAL demonstrated that low field Q slope is caused by amorphous native Nb oxide – host "Two-Level Systems (TLS) losses"
- By eliminating the Nb oxide, we achieved record cavities with $Q_0 > 10^{10}$ in quantum regime (200 times state of the art)



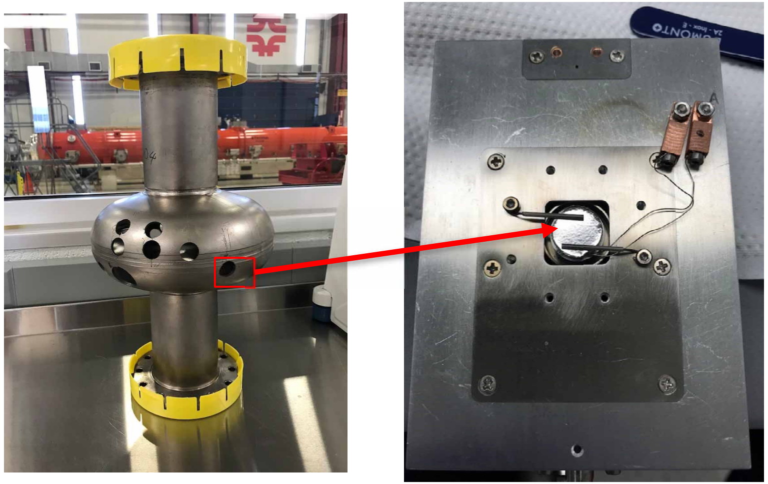
Fermilab discovery of *in situ* mid T bake was driven by these studies to eliminate the Nb pentoxide



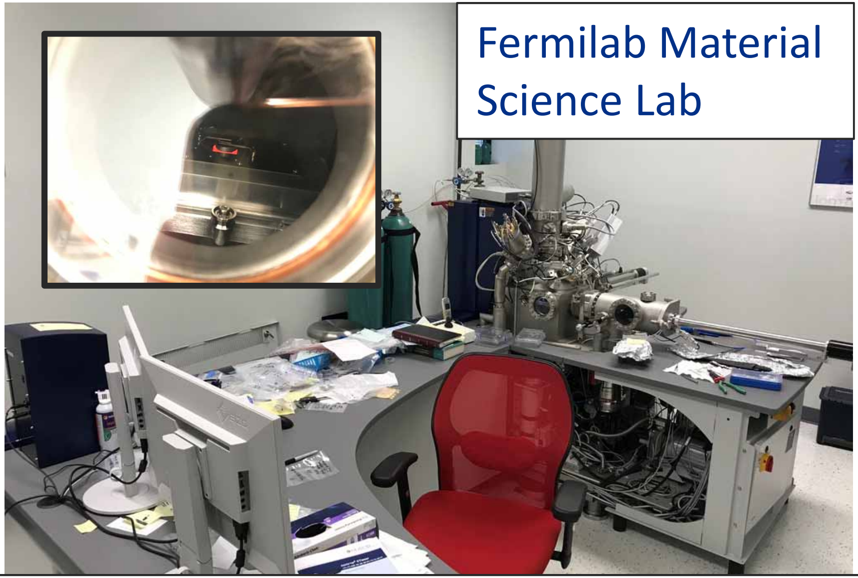


ToF-SIMS was a Key Tool in these studies, driving innovation from the materials

- State-of-the-art FNAL ToF-SIMS enables *in situ* surface processing and depth profiling
- Ability to eliminate particle-induced artifacts from analysis
- Key for the development of mid-T baking



Romanenko, TTC'2020

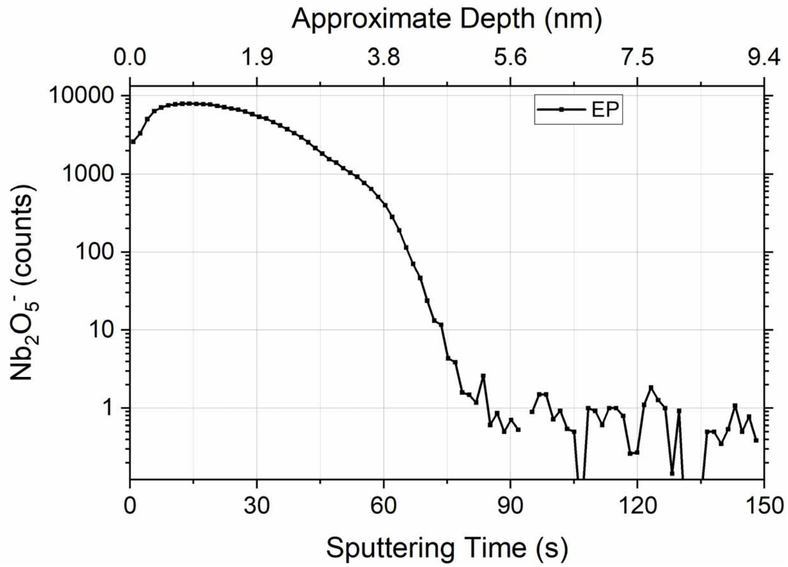


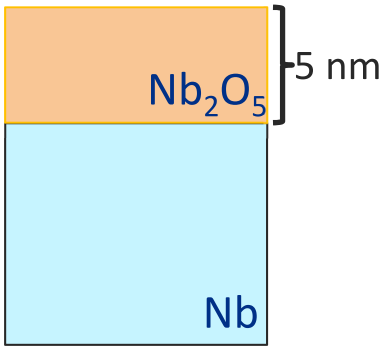
Fermilab Material Science Lab

Equipped w/ Heating Chamber – *in situ* baking studies!

Oxide Evolution Post *in situ* LTB and Mid-T Baking

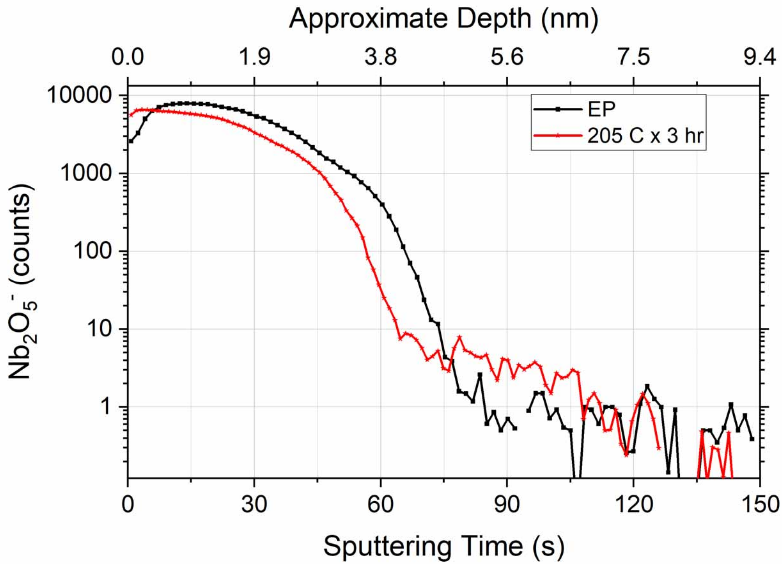
EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C

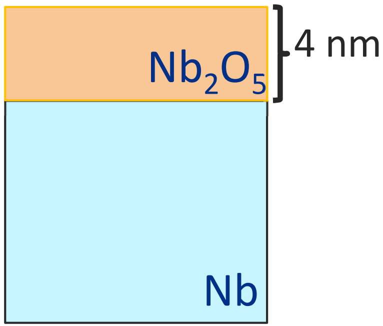




Oxide Evolution Post *in situ* LTB and Mid-T Baking

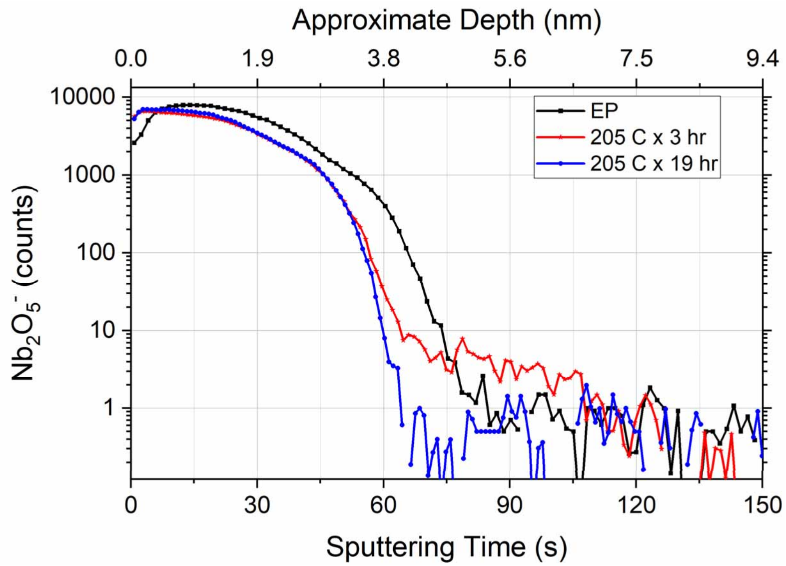
EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C

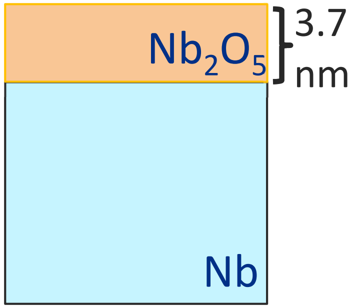




Oxide Evolution Post *in situ* LTB and Mid-T Baking

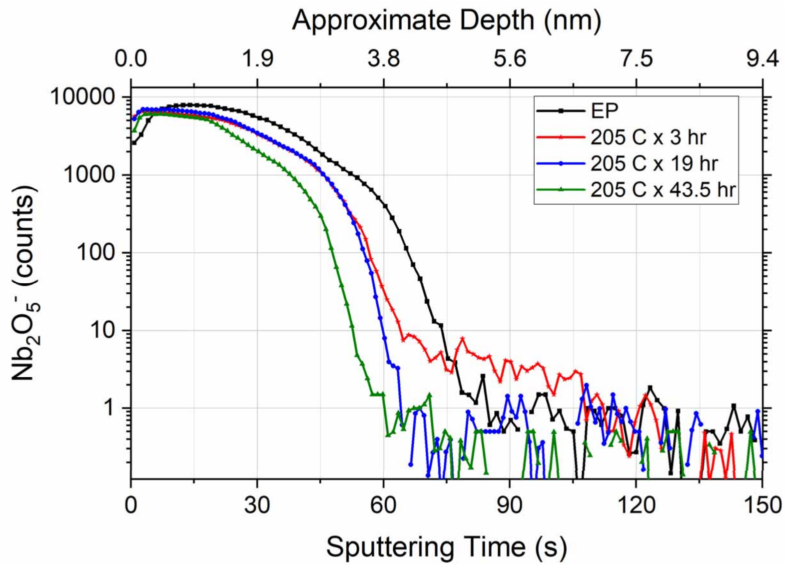
EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C

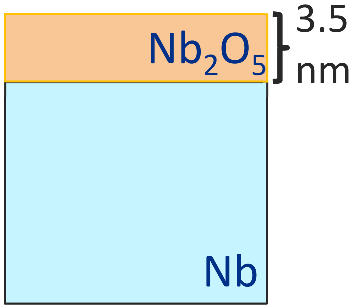




Oxide Evolution Post *in situ* LTB and Mid-T Baking

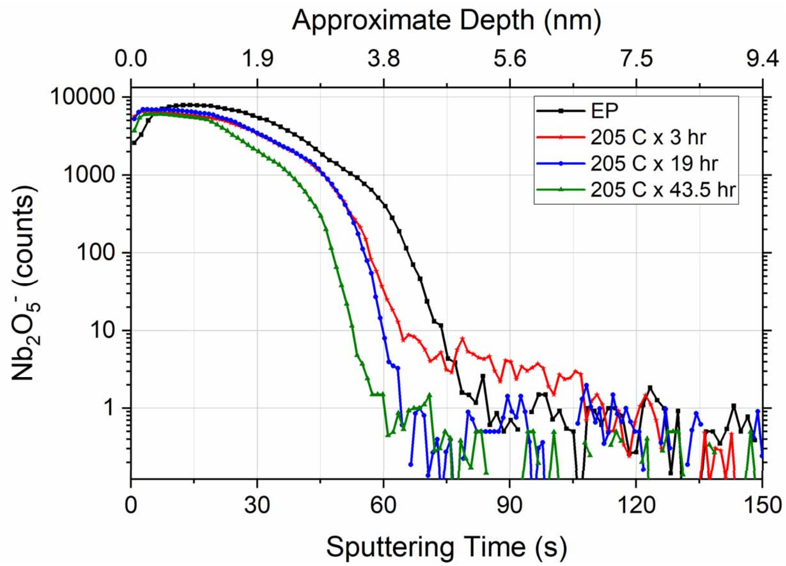
EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C



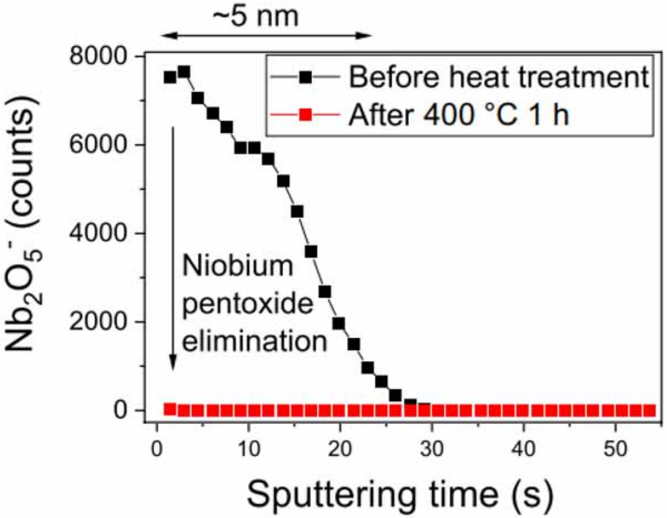


Oxide Evolution Post *in situ* LTB and Mid-T Baking

EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C



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



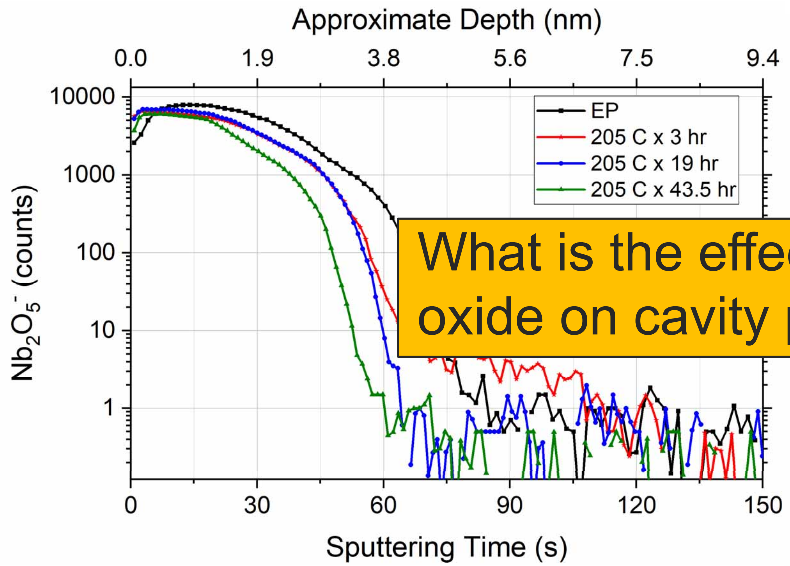
No Nb_2O_5!

- *In situ* LTB at 200 C: partially dissolves Nb_2O_5
- 400C x 1 hr mid-T bake: eliminates Nb_2O_5

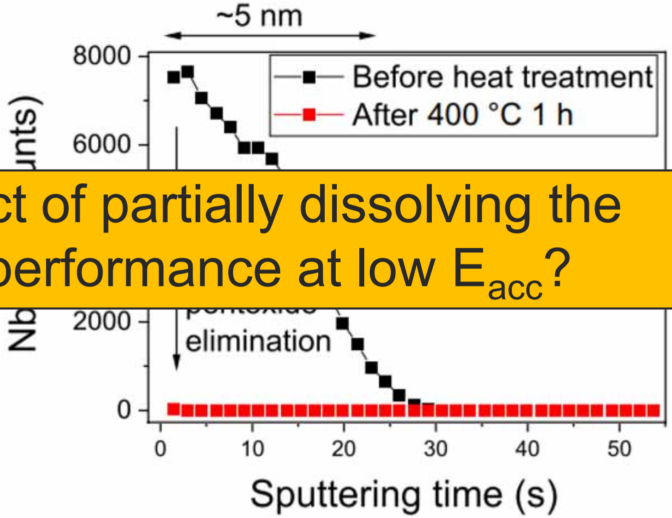
Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Oxide Evolution Post *in situ* LTB and Mid-T Baking

EP cavity cutouts placed into ToF-SIMS and subjected to sequential rounds of *in situ* vacuum baking from 205 C to 400 C



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



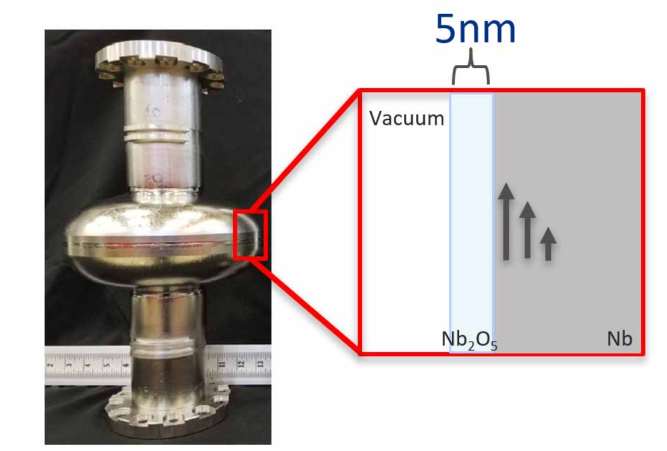
What is the effect of partially dissolving the oxide on cavity performance at low E_{acc}?

No Nb_2O_5!

- *In situ* LTB at 200 C: partially dissolves Nb_2O_5
- 400C x 1 hr mid-T bake: eliminates Nb_2O_5

Study #1: Sequential *in-situ* Vacuum Baking to Identify Source of Low Field Losses

- One Nb cavity was treated to sequential *in situ* vacuum baking and RF tested after each step
- *In situ* vacuum baking: baked fully assembled cavity; maintained evacuated interior volume
  - Vacuum line connected to cavity interior to maintain vacuum (1E-6 Torr)
- Cavity tested at <1.6 K in VTS using decay method with a SA to probe “low” cavity fields



1.3 GHz Nb cavity

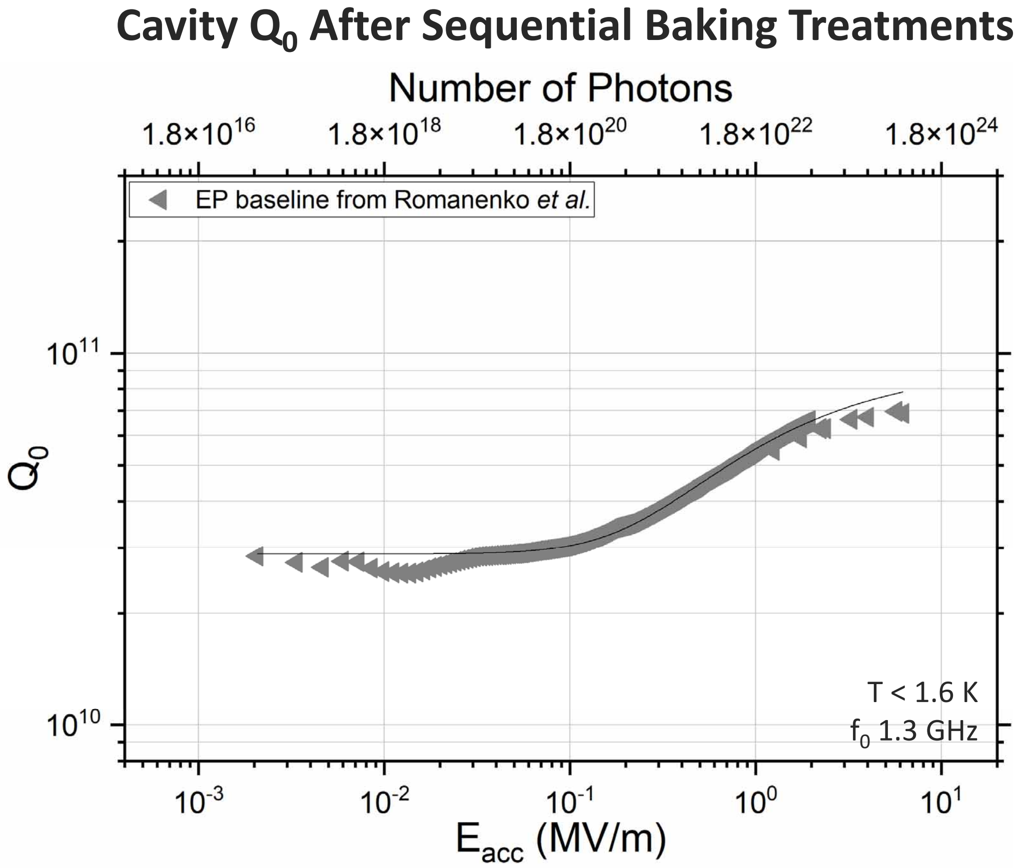
+

Vacuum Baking Treatments
+200 C x 1 hr
+200 C x 5 hrs
+200 C x 5 hrs
+340 C x 5 hrs

Effect of Gradual Vacuum Baking on Cavity Q_0

Baseline:

- Full 5 nm native oxide
- $Q_{0,\text{Low Field}}$ = 2.7E10



Effect of Gradual Vacuum Baking on Cavity Q_0

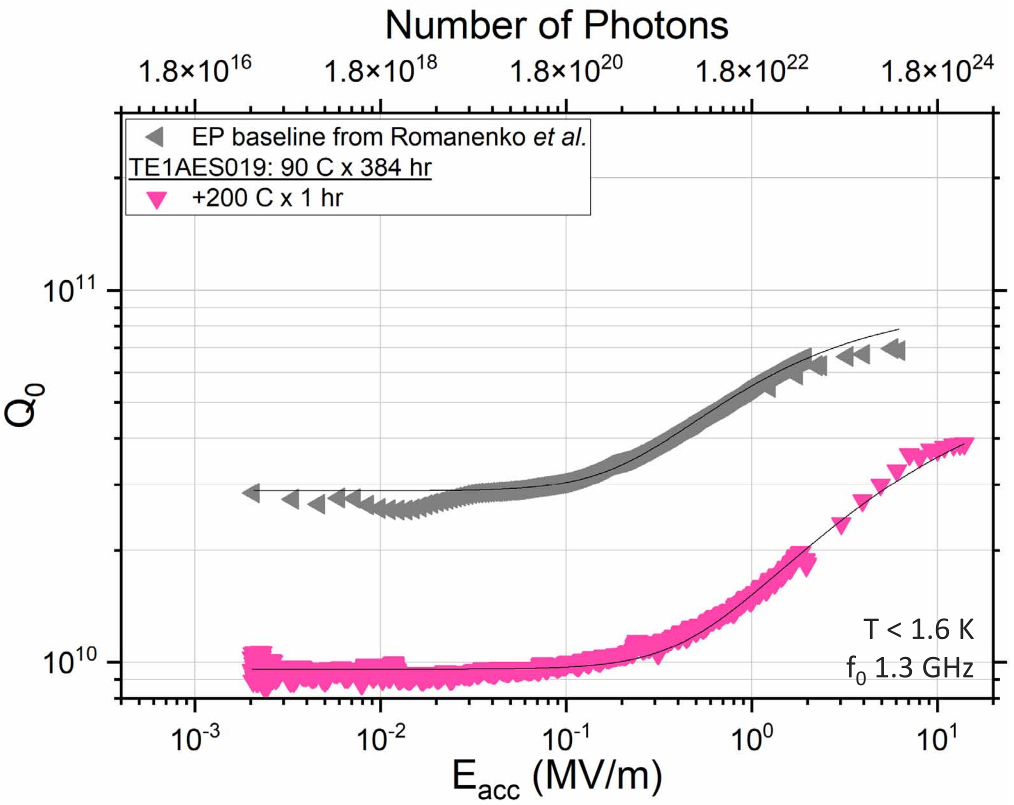
Baseline:

- Full 5 nm native oxide
- $Q_{0,\text{Low Field}}$ = 2.7E10

+200 C x 1 hr:

- $Q_{0,LF}$ decreased by 3x
- **Partially depleting oxide increases the R_{res}**

Cavity Q_0 After Sequential Baking Treatments



Effect of Gradual Vacuum Baking on Cavity Q_0

Baseline:

- Full 5 nm native oxide
- $Q_{0,Low\ Field}$ = 2.7E10

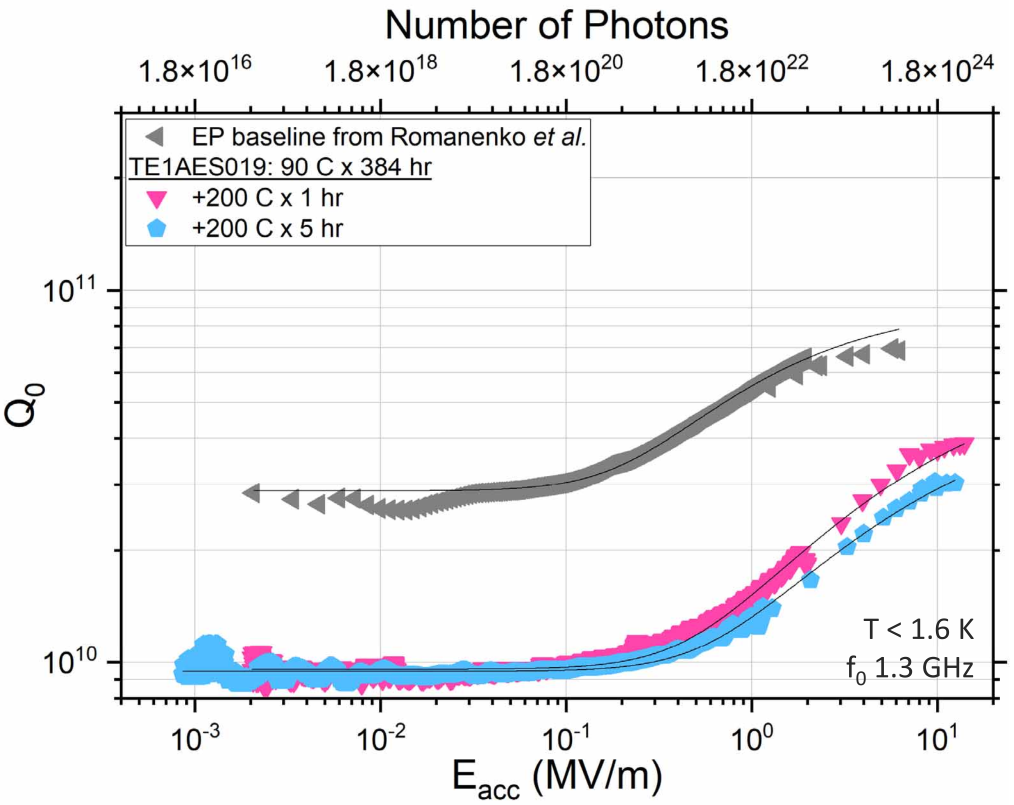
+200 C x 1 hr:

- $Q_{0,LF}$ decreased by 3x
- **Partially depleting oxide increases the R_{res}**

+200 C x 5 hr:

- $Q_{0,LF}$ unchanged

Cavity Q_0 After Sequential Baking Treatments



Effect of Gradual Vacuum Baking on Cavity Q_0

Baseline:

- Full 5 nm native oxide
- $Q_{0,\text{Low Field}}$ = 2.7E10

+200 C x 1 hr:

- $Q_{0,LF}$ decreased by 3x
- **Partially depleting oxide increases the R_{res}**

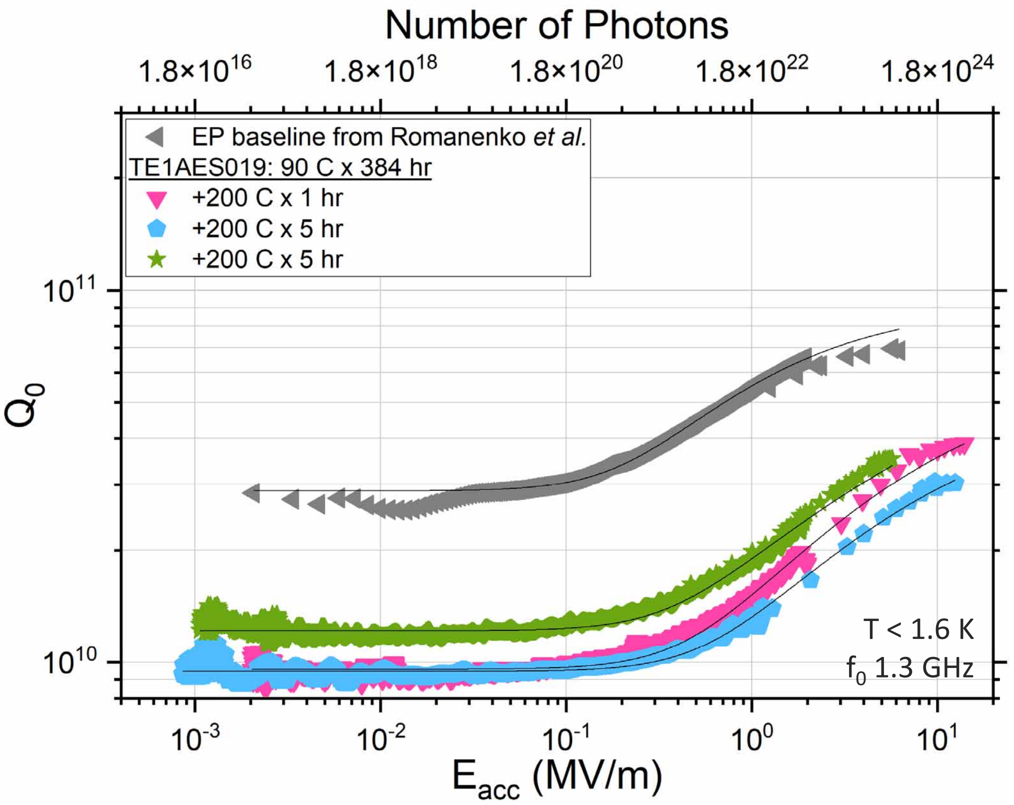
+200 C x 5 hr:

- $Q_{0,LF}$ unchanged

+200 C x 5 hr:

- $Q_{0,LF}$ increased to 1.2E10

Cavity Q_0 After Sequential Baking Treatments



Effect of Gradual Vacuum Baking on Cavity Q_0

Baseline:

- Full 5 nm native oxide
- $Q_{0,\text{Low Field}}$ = 2.7E10

+200 C x 1 hr:

- $Q_{0,LF}$ decreased by 3x
- **Partially depleting oxide increases the R_{res}**

+200 C x 5 hr:

- $Q_{0,LF}$ unchanged

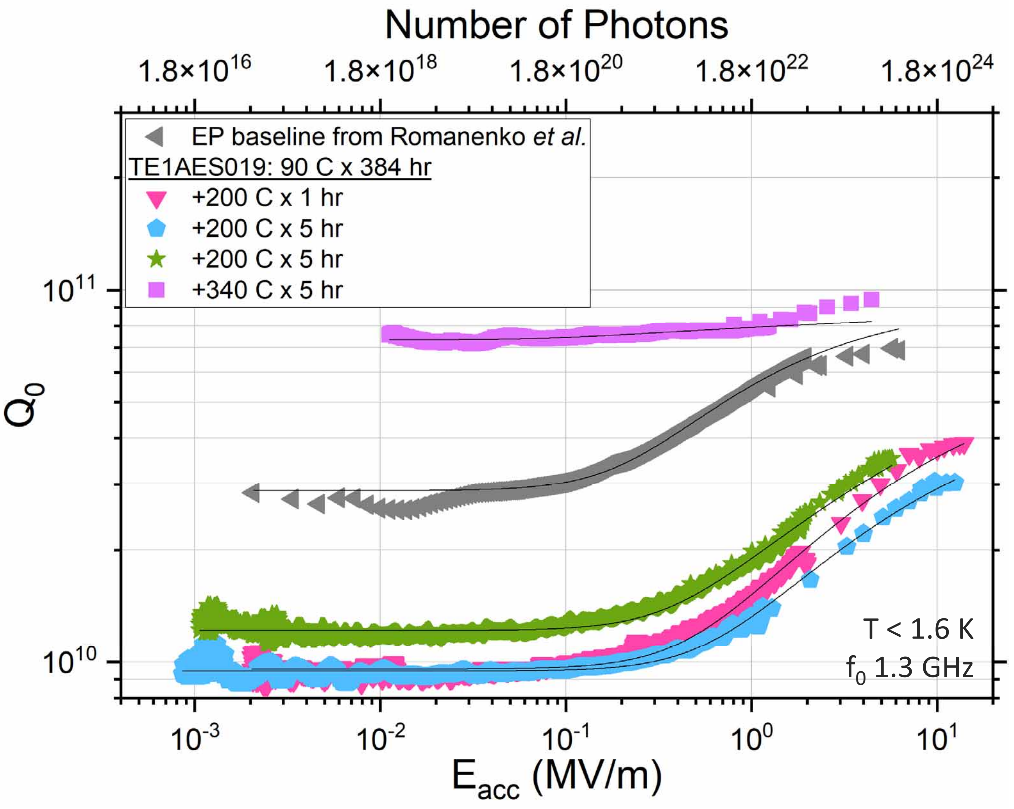
+200 C x 5 hr:

- $Q_{0,LF}$ increased to 1.2E10

+340 C x 5 hr:

- $Q_{0,LF}$ increased by 6x

Cavity Q_0 After Sequential Baking Treatments



Effect of Gradual Vacuum Baking on Cavity Q_0

Baseline:

- Full 5 nm native oxide
- $Q_{0,\text{Low Field}}$ = 2.7E10

+200 C x 1 hr:

- $Q_{0,LF}$ decreased by 3x
- **Partially depleting oxi[de] increases the R_{res}**

+200 C x 5 hr:

- $Q_{0,LF}$ unchanged

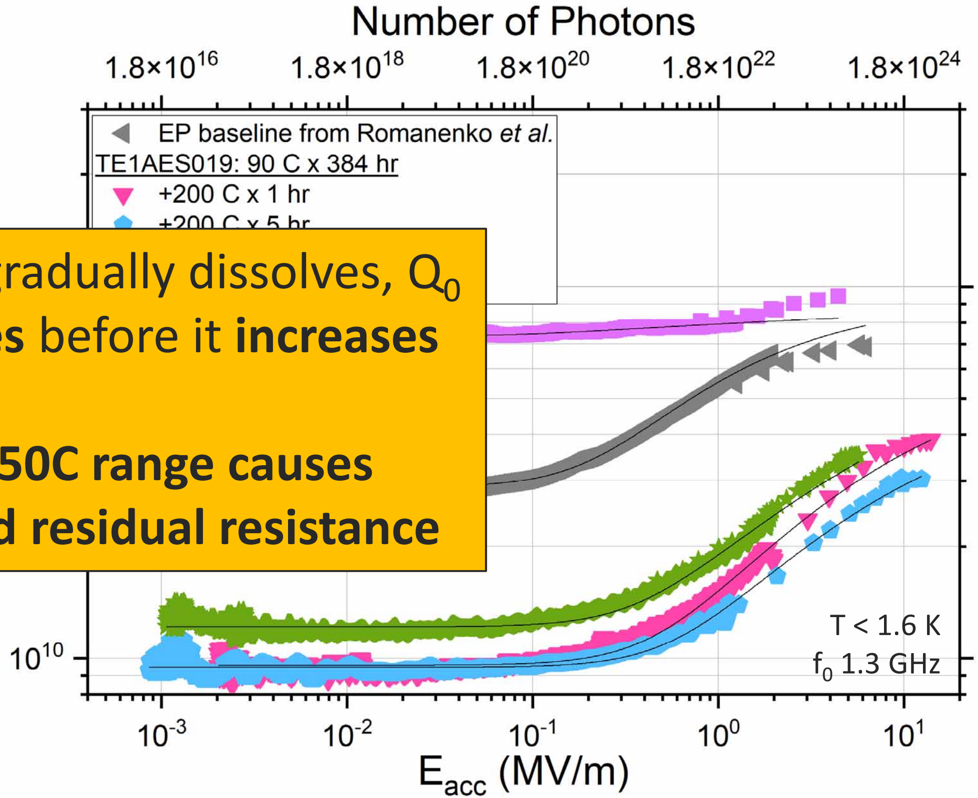
+200 C x 5 hr:

- $Q_{0,LF}$ increased to 1.2E10

+340 C x 5 hr:

- $Q_{0,LF}$ increased by 6x

Cavity Q_0 After Sequential Baking Treatments



As oxide gradually dissolves, Q_0 **decreases** before it **increases**

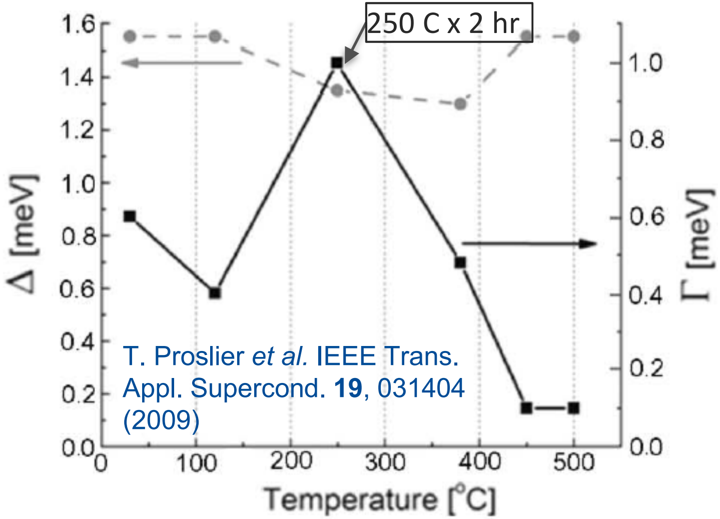
200-250C range causes increased residual resistance

Depleted Oxide as a Source Low Field Loss

- Depleted oxide may host O vacancies in Nb_2O_5
  → Potential magnetic impurities, tunneling sites, ...
  – XAS, DFT: T. Harrelson *et al.* APL **119**, 244004 (2021)

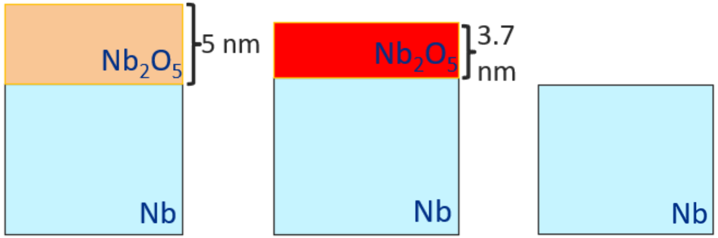
- Vacuum baking dissolves Nb_2O_5, increases # of subgap QP states
  – PCTS: T. Proslier *et al.*

Gap and Dynes Parameters vs Bake Temp of Nb Sample



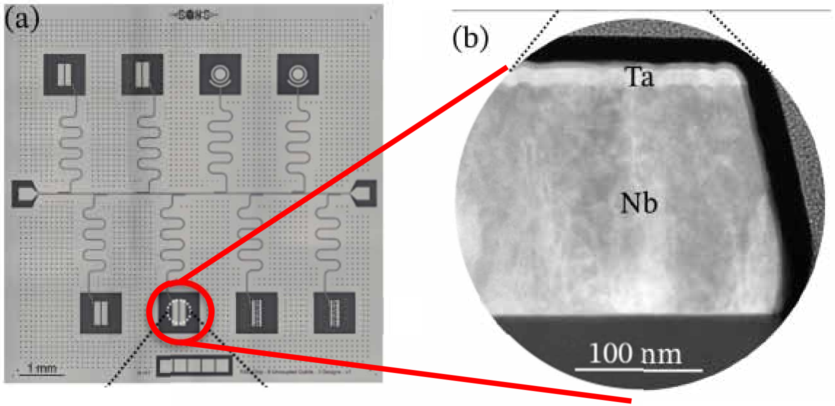
Connection to experimental findings:

- Nonmonotonic Q_0 behavior with baking due to interplay of magnetic suboxide generation and oxide dissolution



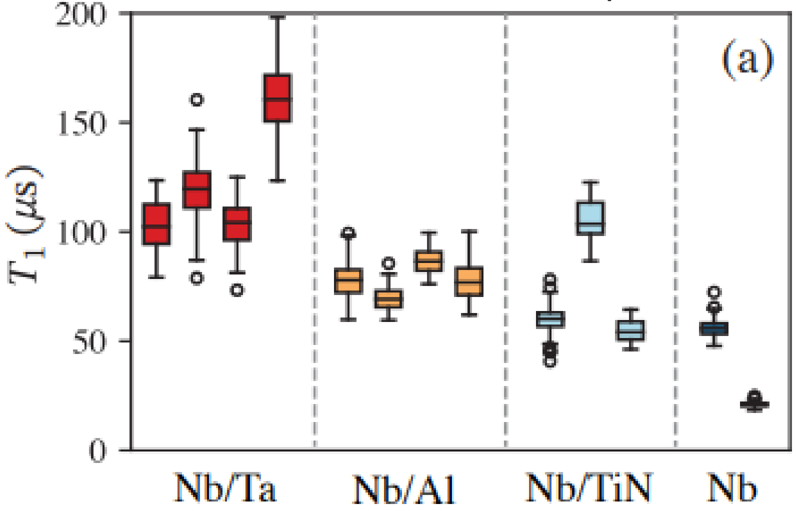
Fermilab Innovation: Preventing Oxidation *via* Niobium Surface Encapsulation

- *In situ* mid-T bake not robust in air
  - Qubits typically require air exposure
- Fermilab developed an encapsulation scheme in which Nb pads are coated with various metals to prevent Nb_2O_5 formation



M. Bal *et al.* arXiv:2304.13257, Submitted to Nature

Nb on Sapphire Qubit Photon Lifetimes Post Various Encapsulations



>2x improvement in T_1 post tantalum encapsulation due to no formation of Nb_2O_5!
At the forefront of qubit coherence!

Fermilab Innovation: Preventing Oxidation *via* Niobium Surface Encapsulation

Nb on Sapphire Qubit Photon

Conclusions From Low Field Studies

- **Oxide drives RF losses in cavities at low fields which are further aggravated by partial oxide dissolution**

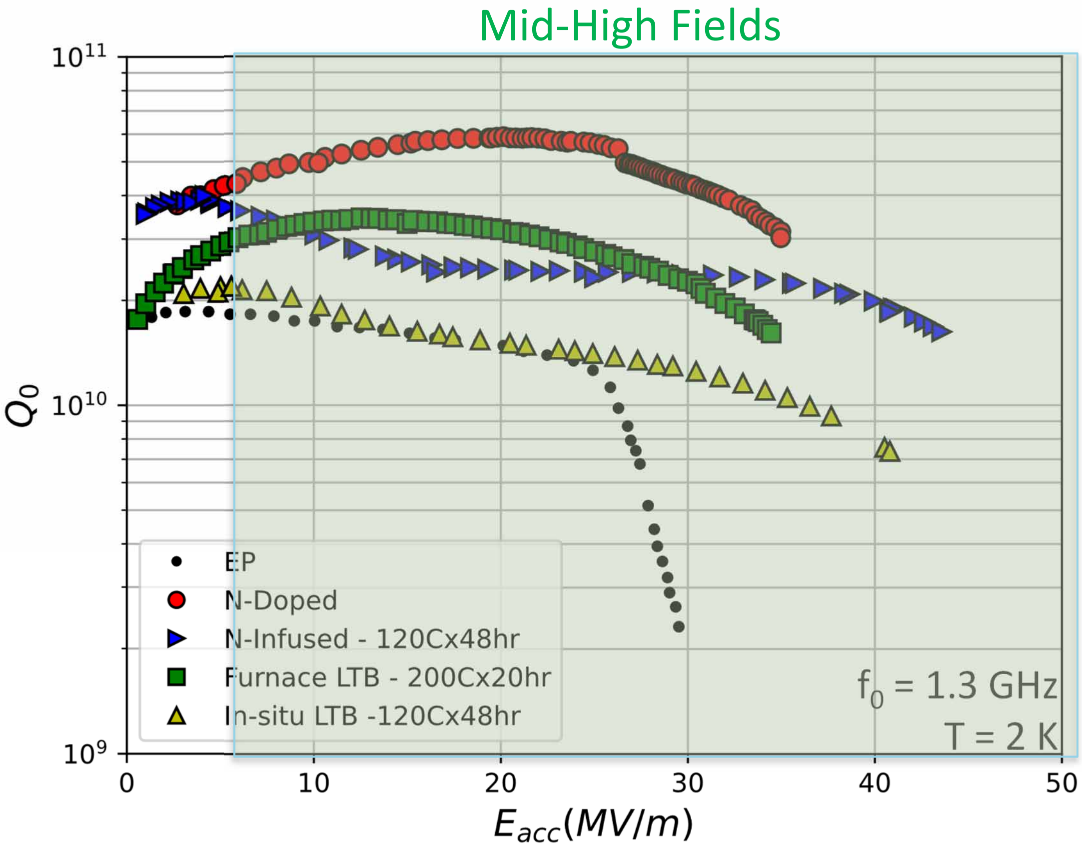
- **Nonmonotonic evolution of Q_0 with baking due to interplay of magnetic suboxide generation and oxide dissolution**

- **Replacing Nb_2O_5 with other potentially less lossy oxides (Tantalum oxide) shows improved photon lifetimes in qubits**

At the forefront of qubit coherence!

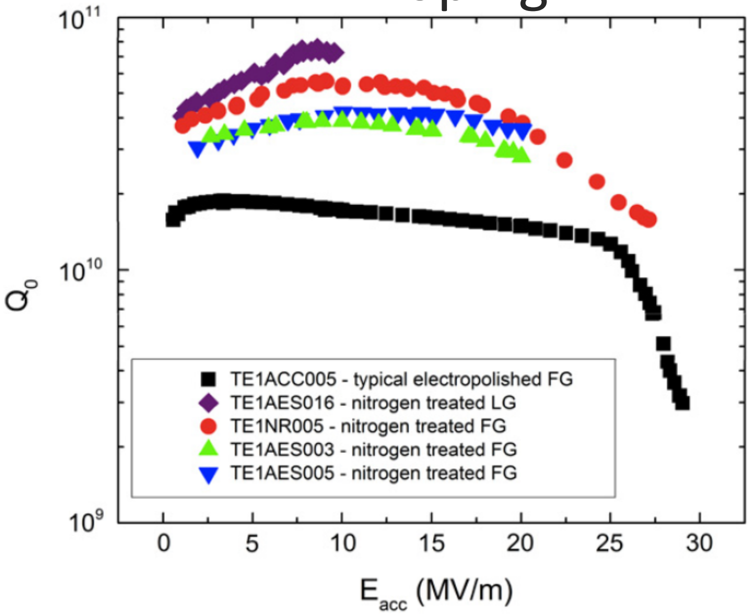
M. Bal *et al.* arXiv:2304.13257, Submitted to Nature

Tailoring Cavity Performance via Surface Processing Techniques



Advancements in Surface Processing Understanding for High E_{acc}

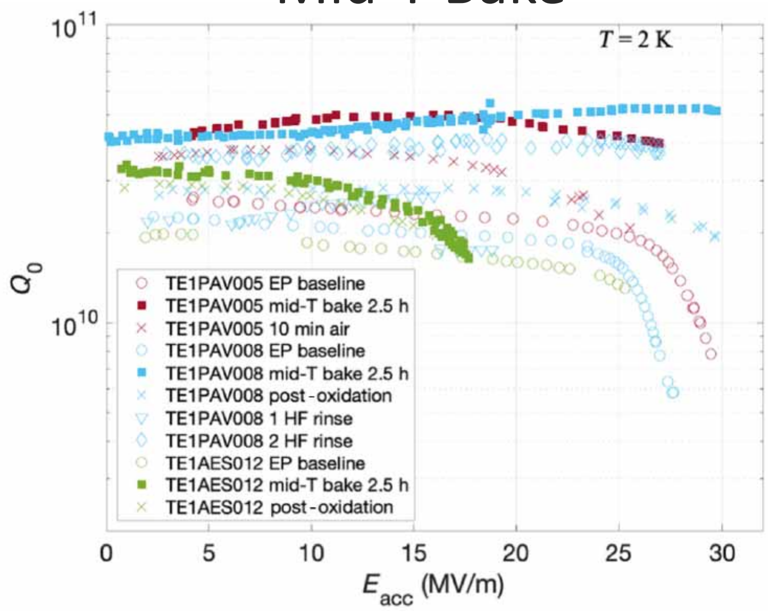
N-Doping



A. Grassellino *et al.*, SUST **26**, 102001 (2013)

Reliably produces high Q_0 and anti-Q slope with **N interstitial**

Mid-T Bake

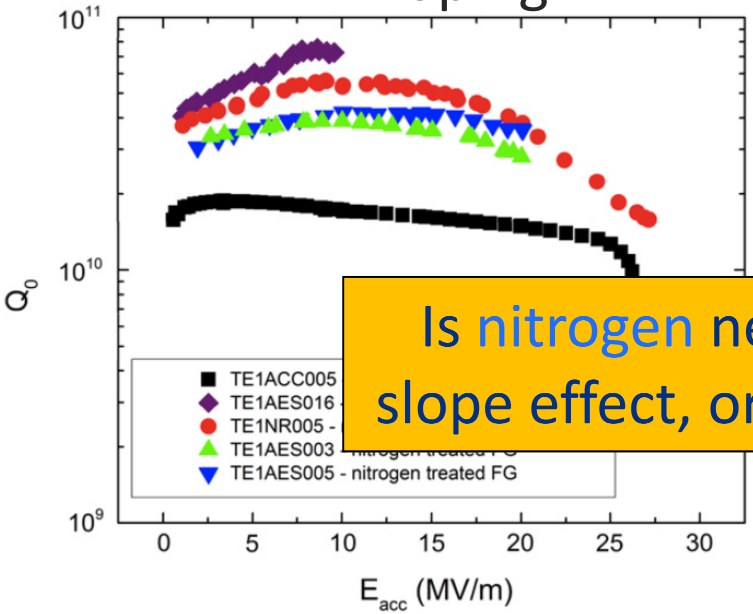


S. Posen *et al.*, PRA **26,** 014024 (2020)

Reliably produces high Q_0 and anti-Q slope with **N** and **O interstitial**

Advancements in Surface Processing Understanding for High E_{acc}

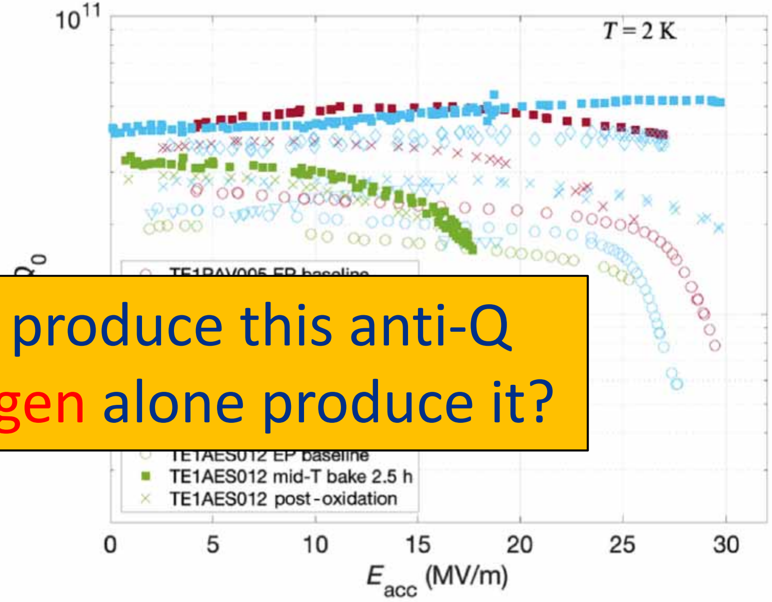
N-Doping



A. Grassellino *et al.*, SUST **26**, 102001 (2013)

Reliably produces high Q_0 and anti-Q slope with **N interstitial**

Mid-T Bake



S. Posen *et al.*, PRA **26,** 014024 (2020)

Reliably produces high Q_0 and anti-Q slope with **N** and **O interstitial**

Is nitrogen needed to produce this anti-Q slope effect, or can oxygen alone produce it?

Study #2: Decoupling N and O in Driving the Anti-Q Slope Effect

- One 1.3 GHz SRF single-cell cavity was subjected to sequential rounds of *in-situ* low temperature baking at 90 C - 200 C and tested after each step
- Cavity maintained vacuum throughout entire study

1.3 GHz single cell

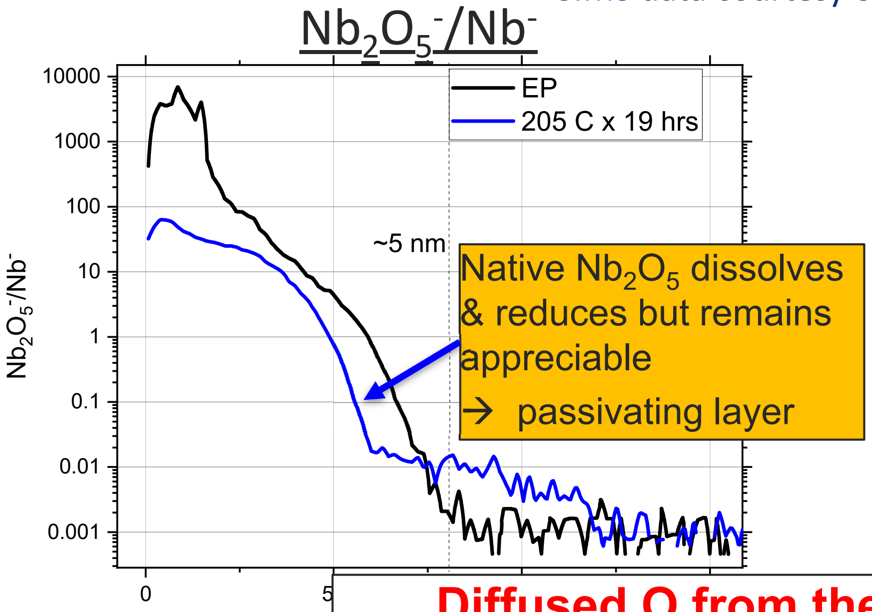
+

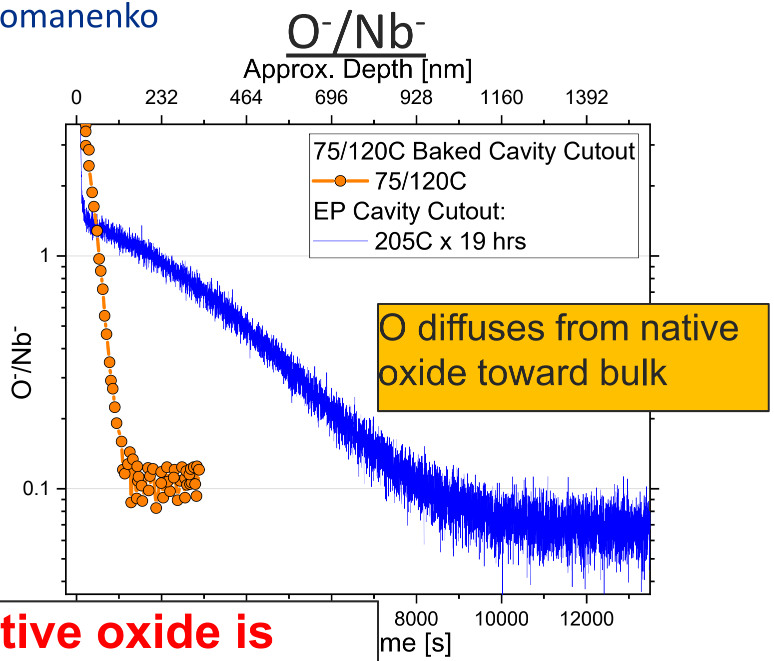
Low Temperature Bake
90 C x 12 hours
+90 C x 384 hours
+200 C x 1 hours
+200 C x 11 hours

O is Primary Diffusant of Interest for These Baking Treatments

EP Nb cavity cutouts were studied with TOF-SIMS after *in-situ* baking

SIMS data courtesy of A. Romanenko





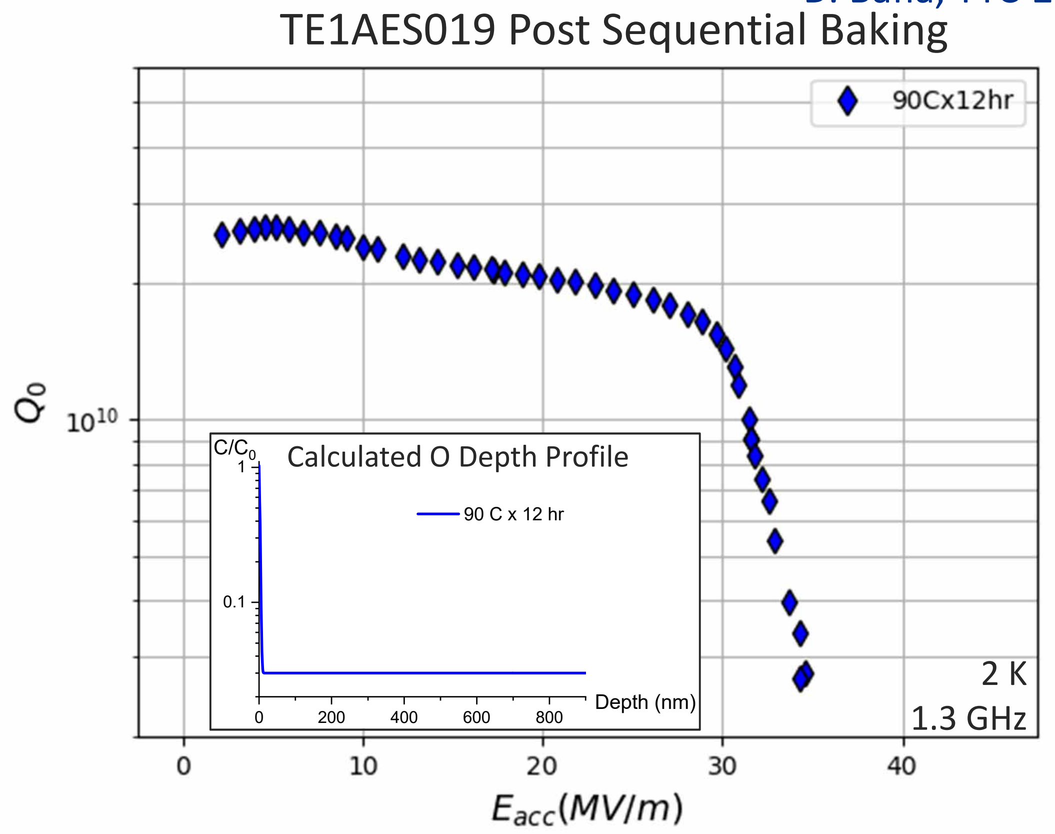
Diffused O from the native oxide is responsible for the following observations

Effect of Oxygen Diffusion on Mid-High Field Performance

Cavity maintained vacuum throughout entire study

- **90 C x 12 hr**
  - HFQS

D. Bafia, TTC'22

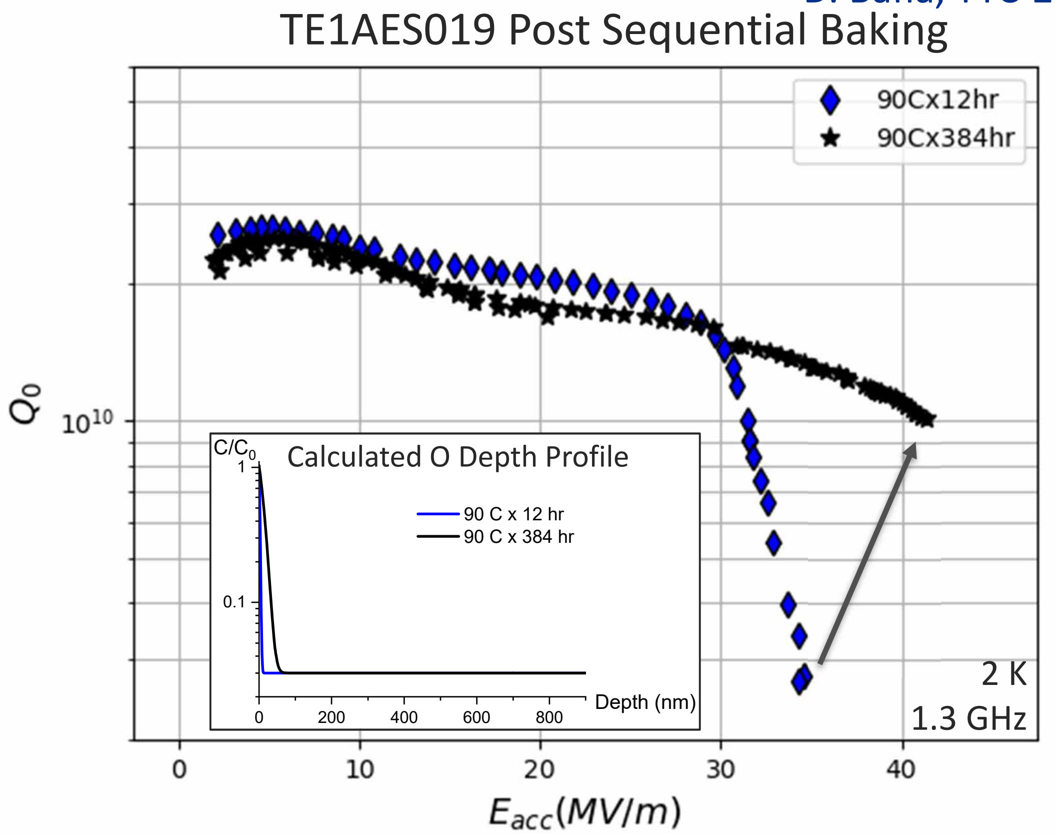


Effect of Oxygen Diffusion on Mid-High Field Performance

D. Bafia, TTC'22

Cavity maintained vacuum throughout entire study

- **90 C x 12 hr**
  - HFQS
- **90 C x 384 hr**
  - Diffuses oxygen ~64 nm, no HFQS up to quench

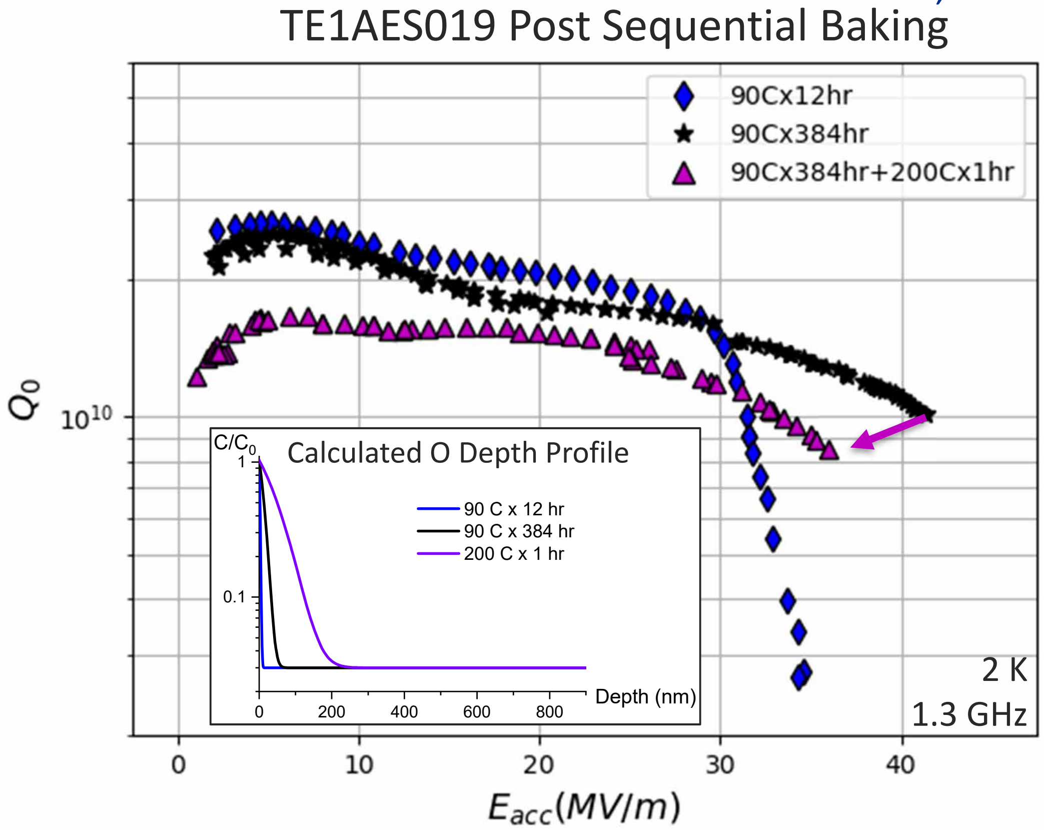


Effect of Oxygen Diffusion on Mid-High Field Performance

Cavity maintained vacuum throughout entire study

- **90 C x 12 hr**
  - HFQS
- **90 C x 384 hr**
  - Diffuses oxygen ~64 nm, no HFQS up to quench
- **200 C x 1 hr**
  - Rounding of curve

D. Bafia, TTC’22

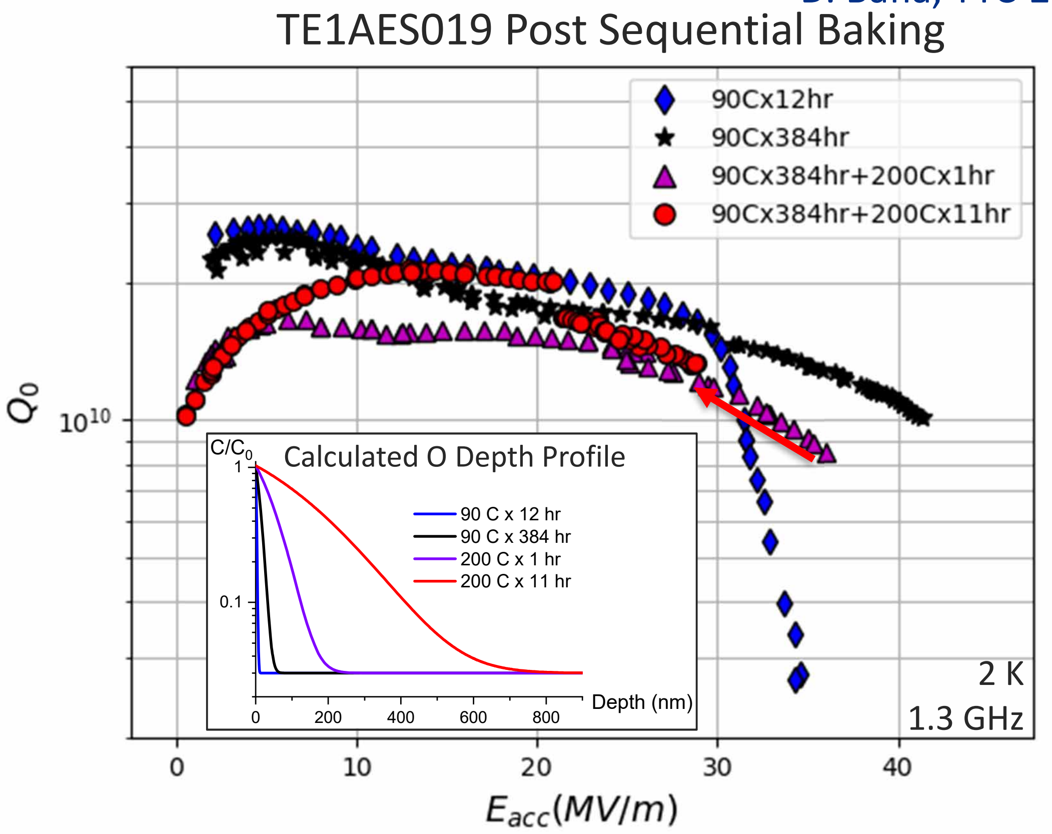


Effect of Oxygen Diffusion on Mid-High Field Performance

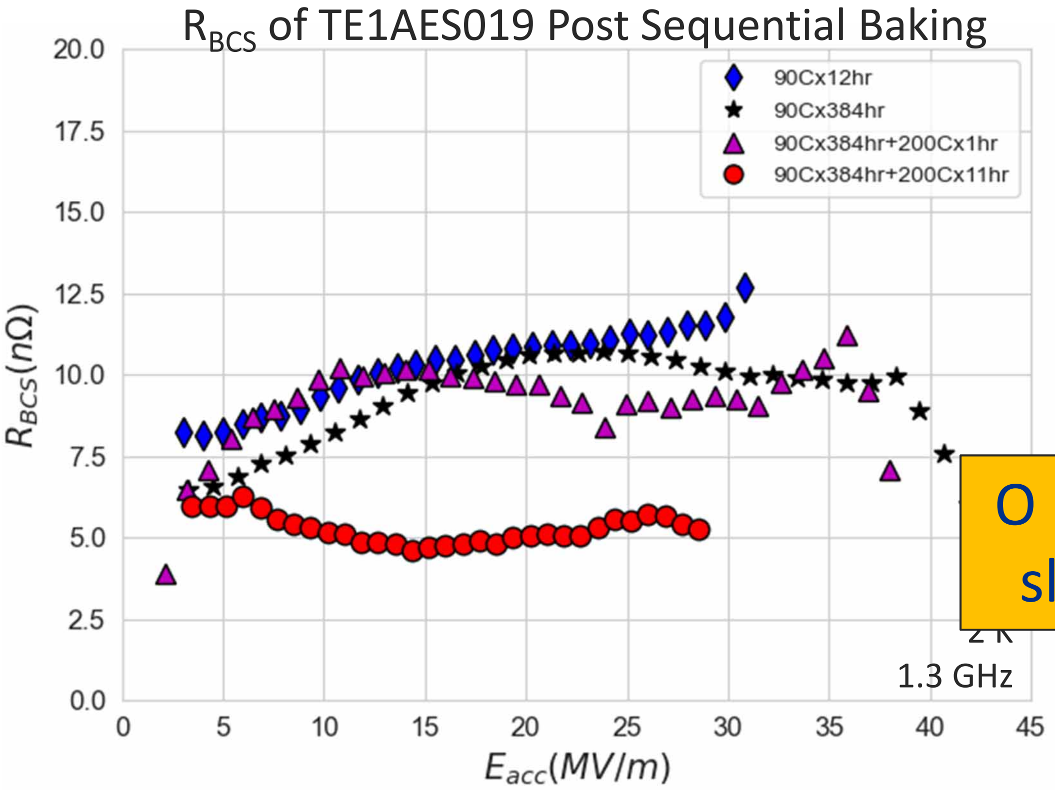
Cavity maintained vacuum throughout entire study

- **90 C x 12 hr**
  - HFQS
- **90 C x 384 hr**
  - Diffuses oxygen ~64 nm, no HFQS up to quench
- **200 C x 1 hr**
  - Rounding of curve
- **200C x 11 hr**
  - Anti-Q slope→ **"O-Doped?"**

D. Bafia, TTC'22



Effect of Oxygen Diffusion on BCS Resistance



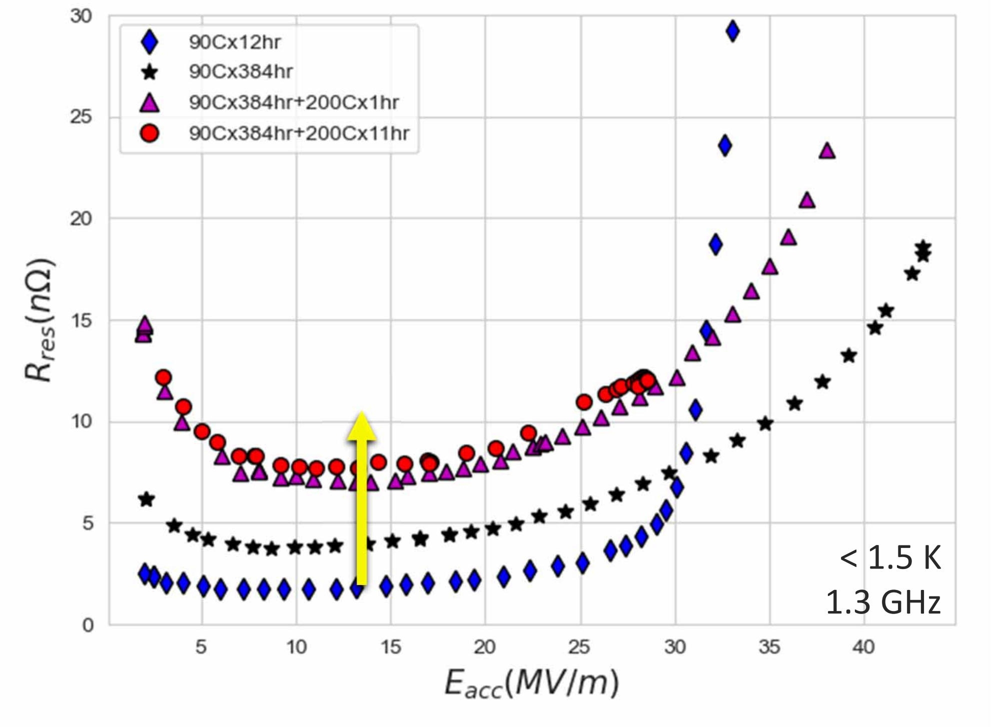
Introducing more oxygen gradually causes an overall reduction in the R_{BCS}

O impurities alone drive anti-Q slope in *in situ* baked cavities

Effect of Oxygen Diffusion on Residual Resistance @ High E_{acc}

- TE1AES019 underwent *in-situ* vacuum baking without ever losing vacuum
  - Never reformed native oxide
- With each step of baking:
  - R_{res} increased
- Evolution of R_{res} is again explained by the gradual dissolution of the native niobium oxide

R_{res} of TE1AES019 Post Sequential Baking



Subtracted off trapped flux introduced at 15 MV/m

Effect of Oxygen Diffusion on Residual Resistance @ High E_{acc}

Conclusions from High Field Studies

- Oxygen alone can drive high Q_0 and anti-Q slope post *in situ* LTB
  – Uniform and dilute concentrations of O = O-doping
  – Diffusion depth critical to obtain different Q and quench fields
- 10 years ago, we had no way of varying mid-field and high performance (only 120C bake), now we understand that have two different ways: N or O
- Charge for future work: are there collaborative effects between N AND O?

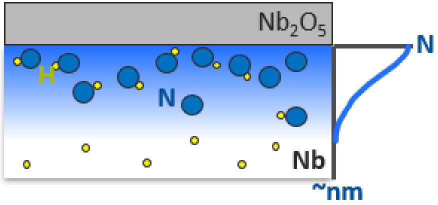
Putting It All Together: Summary of Surface Treatments

N Focused Treatments

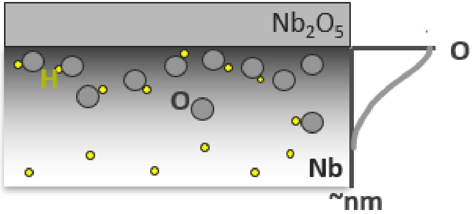
Vacuum/O Focused Treatments

Low Temperature (90 C – 200 C)

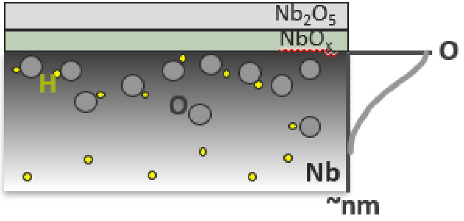
N-Infusion



Furnace LTB



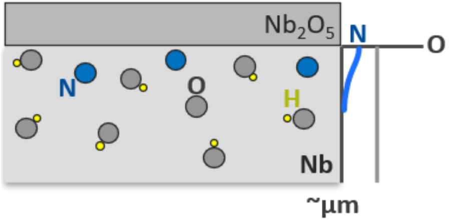
In Situ LTB



Mid Temperature (300 C < T < 450 C)

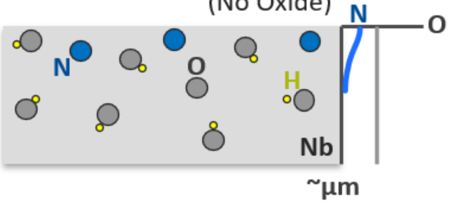
Under exploration

Furnace Mid-T Bake



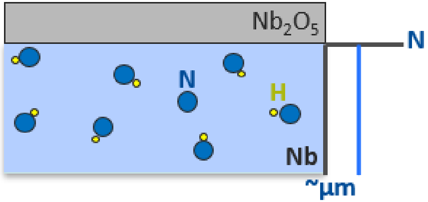
In situ Mid-T Bake

(No Oxide)

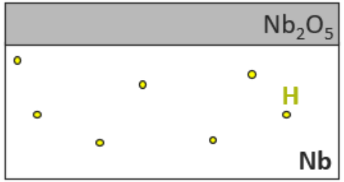


High Temperature (+700 C)

N-Doping



800C HT Baked



No extrinsic impurities

Conclusions

Low Fields

- Synergistic accelerator and quantum computing R&D shows that oxides drive low field losses which are aggravated by partial oxide dissolution
  - Nonmonotonic evolution of Q_0 with successive baking due to interplay of oxygen depleted oxide, magnetic suboxide generation and overall oxide thickness reduction

High Fields

- Both N and O are key impurities which enable excellent cavity performance
  - High gradient, High Q, and anti-Q slope
- **Do we still need N?**
  - For now, yes → Excellent cavity performance after a decade of R&D in N-Doping, and still room for improving accelerating gradients further
  - BUT: continued optimization (trapped flux sensitivity and reproducibility) of O-doping and Mid-T baking recipes may reveal similar advancements

Acknowledgements

- This work has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics
- This material is based upon work supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS) under contract number DE-AC02-07CH11359

Thank you for your attention!