Enhanced RF Performances in 1.3 GHz Nb Cavities via Mid-T Baking: Insights from Correlative Sample Studies

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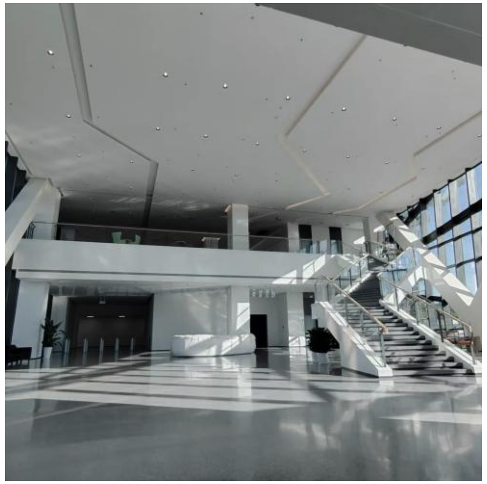
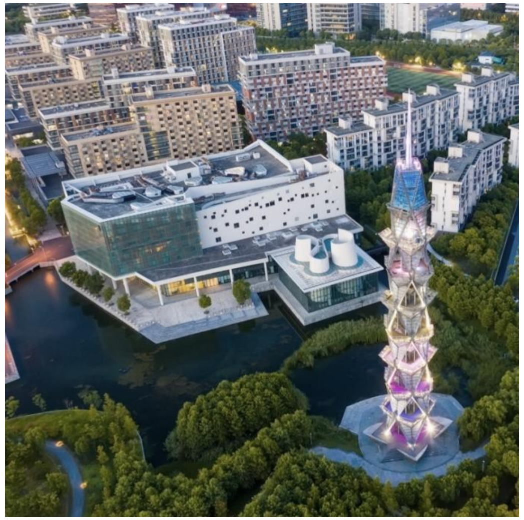
On behalf of collaboration team at SHINE

2026.6.10

Shanghai **HI**gh repetitio**N** rate XFEL and **E**xtreme light facility (**SHINE**)





ShanghaiTech Campus

Co-Construction: SARI, SIOM

Project Funding: 10.436 billion CNY

Commencement Date: April, 2018

Outlines

1. **Mid-T baking treatment at SHINE**
    a) Procedures
    b) SRF performance (1.3 GHz cavities)
2. **Sample coupon studies**
    a) XPS studies
    b) SIMS studies
    c) Microscopy studies
3. **Insights on the SRF performance improvement**

Collaborations on SRF materials R&D

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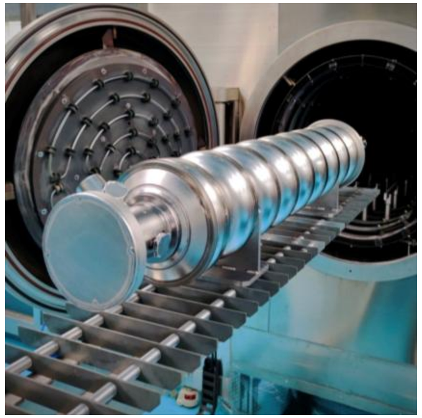
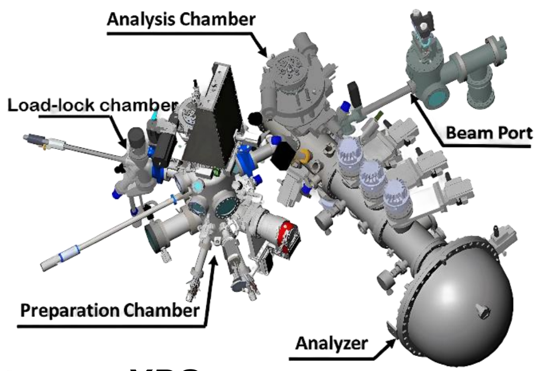


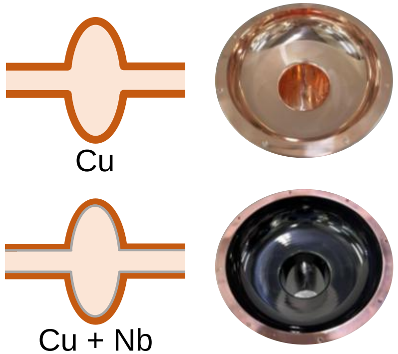
Materials Characterizations

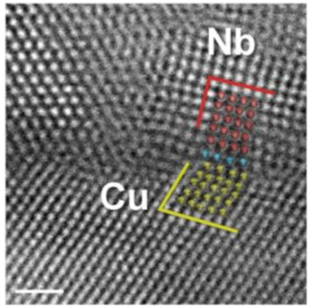


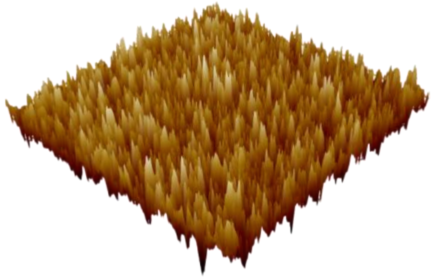
XPS

SIMS; AES; SEM

AC-TEM







上海科技大学
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SHINE

中国科学院上海高等研究院
SHANGHAI ADVANCED RESEARCH INSTITUTE, CHINESE ACADEMY OF SCIENCES

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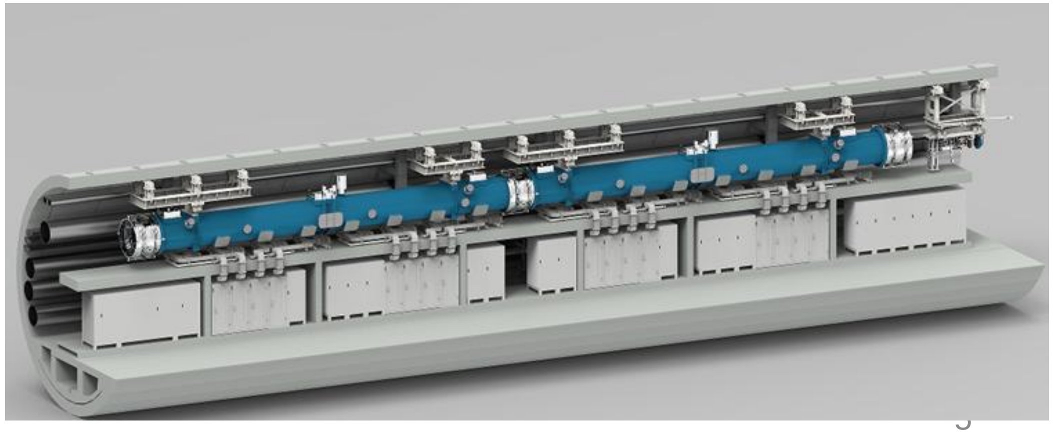
Motivations for High Q_0 & E_{acc}

Updated Requirements for High-Q Cavities and CMs

	1.3 GHz high-Q Cavity		1.3 GHz high-Q CM	
	Bef. Oct 2024	**Now (updated)**	**Bef. Oct 2024**	**Now (updated)**
Amount	600	> 432	75	54 (+4 spare)
Q_0 (10^{10})	≥ 2.7 @16 MV/m	**≥ 3.0 @20 MV/m**	≥ 2.7@16MV/m	**≥ 3.0 @ 20 MV/m**
Max E_{acc}	≥ 19 MV/m	**≥ 22 MV/m**		26 MV/m(adm. limit)
Total voltage			≥ 128 MV	≥ 166 MV

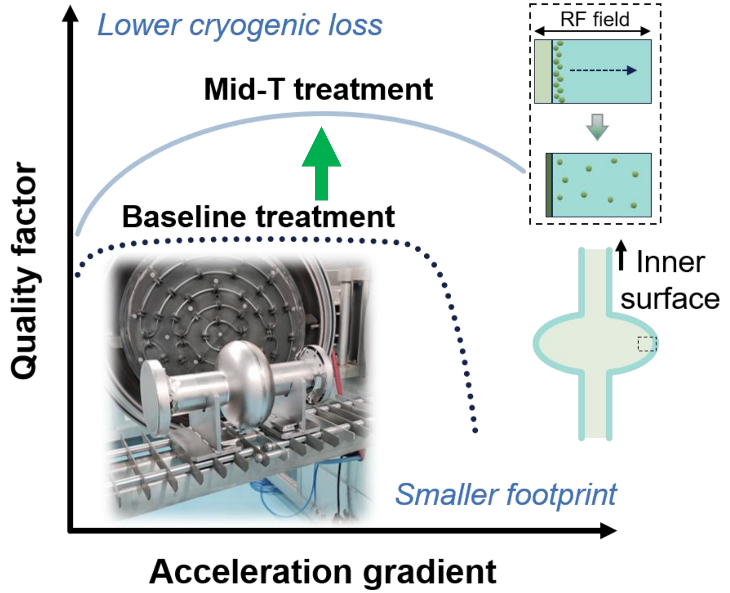


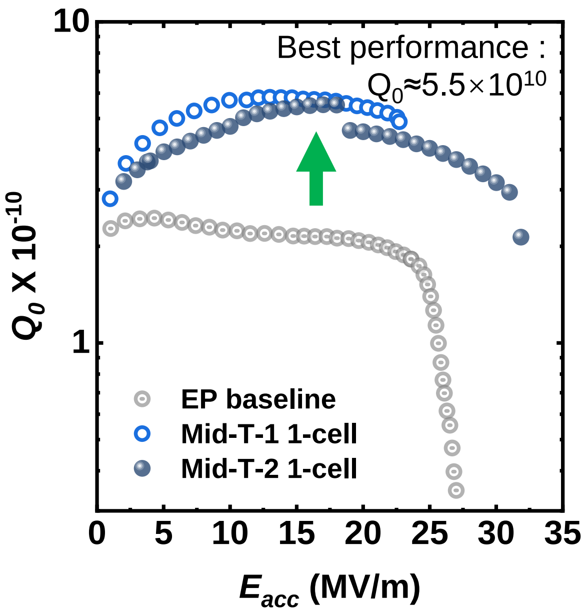
Mid-T baking – recipe

Mid-T baking

Mid-T-1: EP → High temperature baking → EP → Mid-T baking → HPR+Assembly → VT

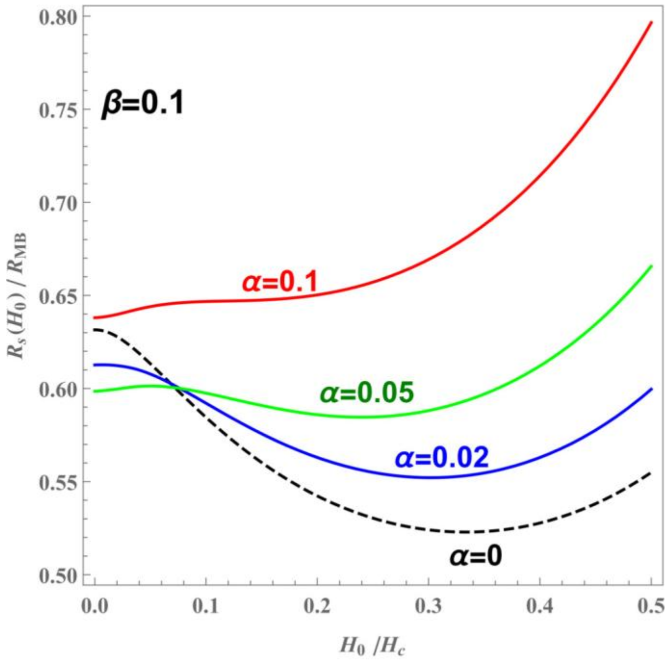
Mid-T-2: EP → High temperature baking → Exposure to air → Mid-T baking → HPR+Assembly → VT





- Mid-T baking requires no intentional gas feeding or post-bake material removal.
- Mid-T-1: The final 300°C baking is performed after electropolishing, which resets the surface oxide layer.
- Mid-T-2: **No intermediate electropolishing** after the 900 °C treatment. The surface retains chemical modifications introduced during high-temperature annealing.

Interface contributions? Shifts of minimum surface resistance to higher fields

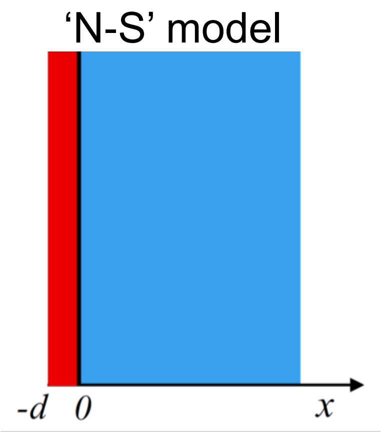


PROXIMITY COUPLED NORMAL LAYER AT THE SURFACE

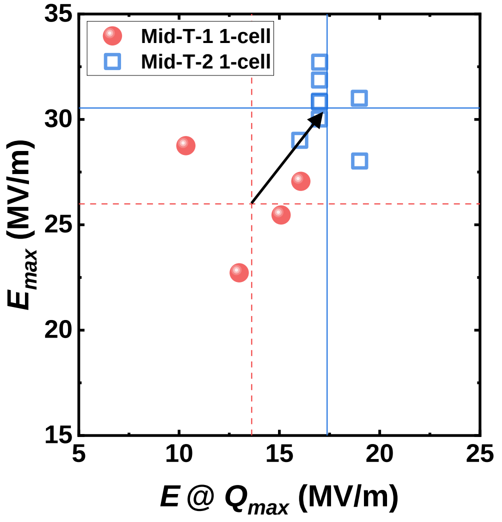
Interface parameters:

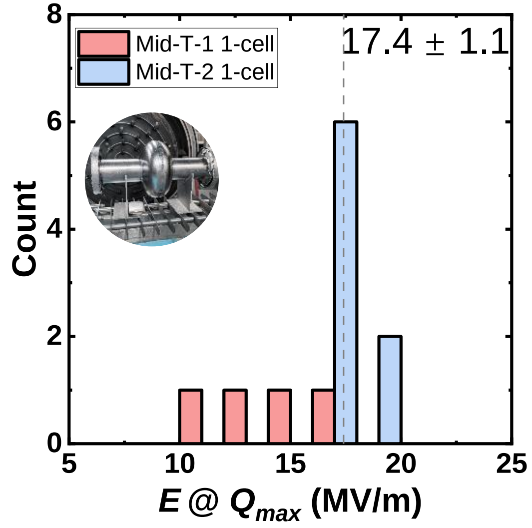
$$\alpha = \frac{N_n}{N_s}\frac{d}{\xi_s},$$

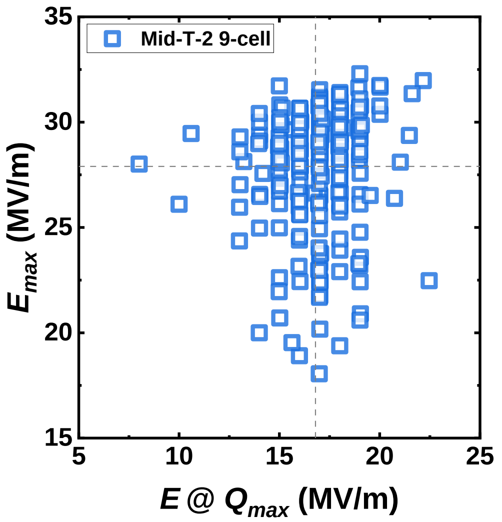
$$\beta = \frac{4e^2}{\hbar}R_B N_n \Delta d,$$

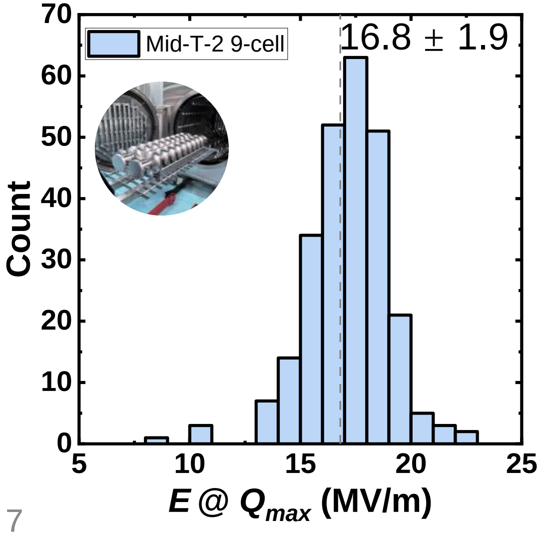


In addition to interstitials, oxide overlayers are modified during Mid-T baking.









PHYSICAL REVIEW B 100, 064522 (2019)

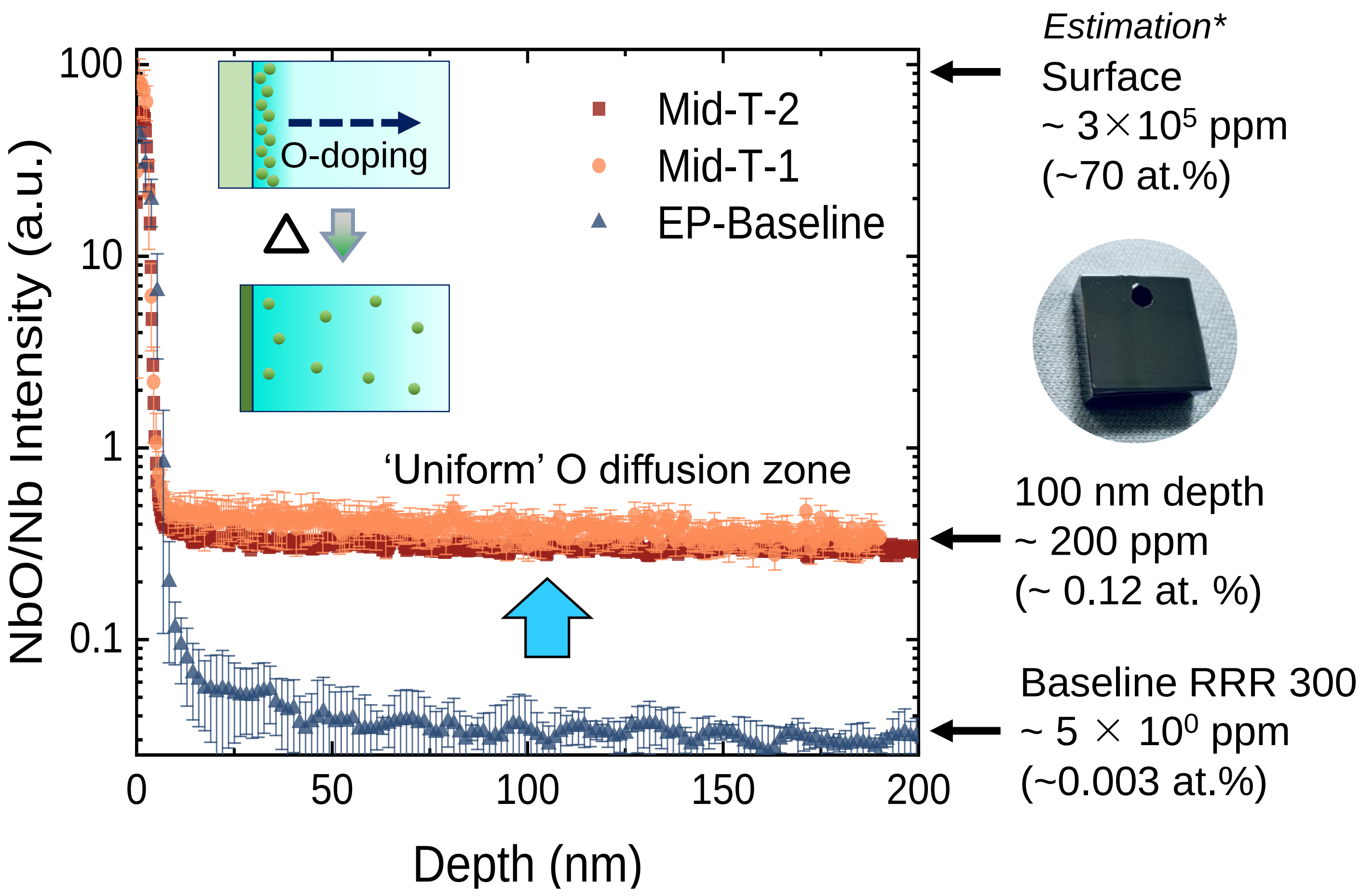
Characterization strategies

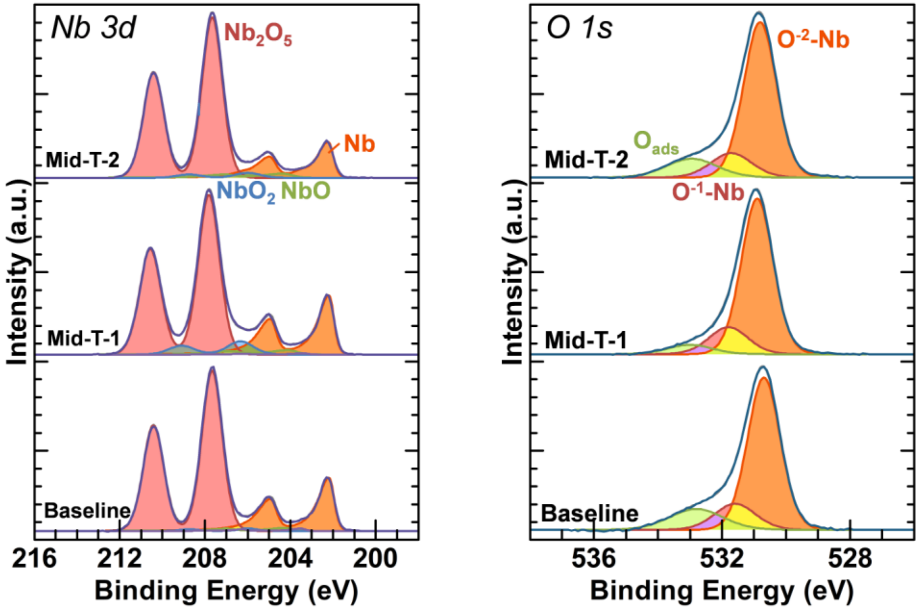
The study uses a correlative approach to connect RF performance with atomic-scale interfacial chemistry.

- **X-ray photoelectron spectroscopy, XPS**
  - Determines surface chemical states of Nb, O, and C.
  - Identifies Nb oxidation states: Nb^0, Nb^{2+}, Nb^{4+}, Nb^{5+}.
  - Tracks oxide dissolution and suboxide evolution.
- **In situ XPS**
  - Monitors thermal evolution of surface oxides during annealing.
  - Reveals temperature-dependent formation and dissolution of NbO-like species.
- **Time-of-flight secondary ion mass spectrometry, TOF-SIMS**
  - Provides depth profiles of O, C, H, NbO, NbC, NbH, NbN-related species.
  - Resolves impurity distributions over the first tens to hundreds of nanometers.
- **Transmission electron microscopy and 4D-STEM**
  - Reveals nanoscale morphology, interfacial strain, dislocations, and oxide-related lattice distortion.
- **Scanning tunneling microscopy/spectroscopy, STM/STS**
  - Probes local superconducting density of states.
  - Extracts superconducting gap Δ and Dynes broadening parameter Γ.

Mid-T baking – O doping

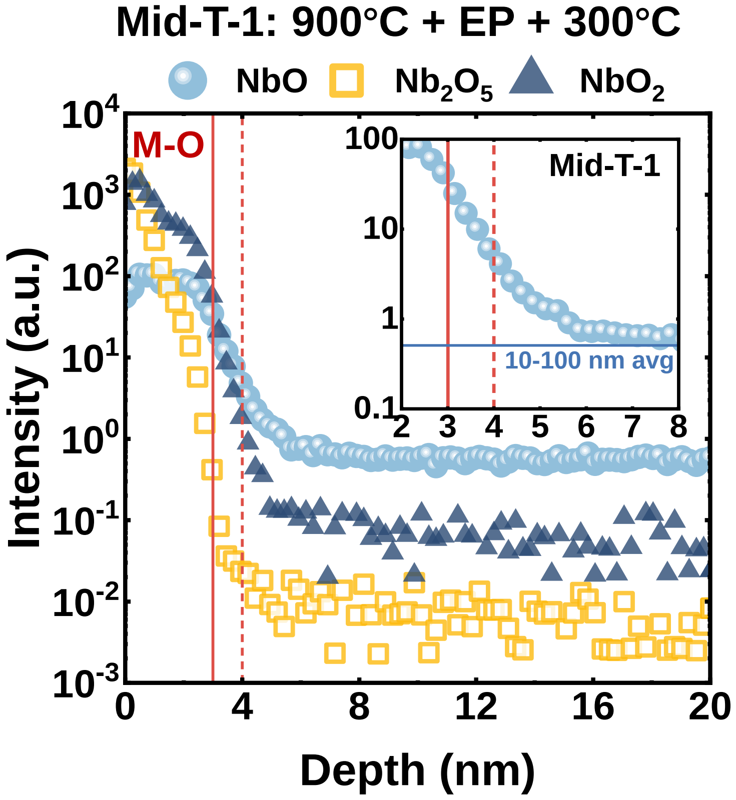
Mid-T-1: 900°C + EP + 300°C **Mid-T-2: 900°C + air exp + 300°C**

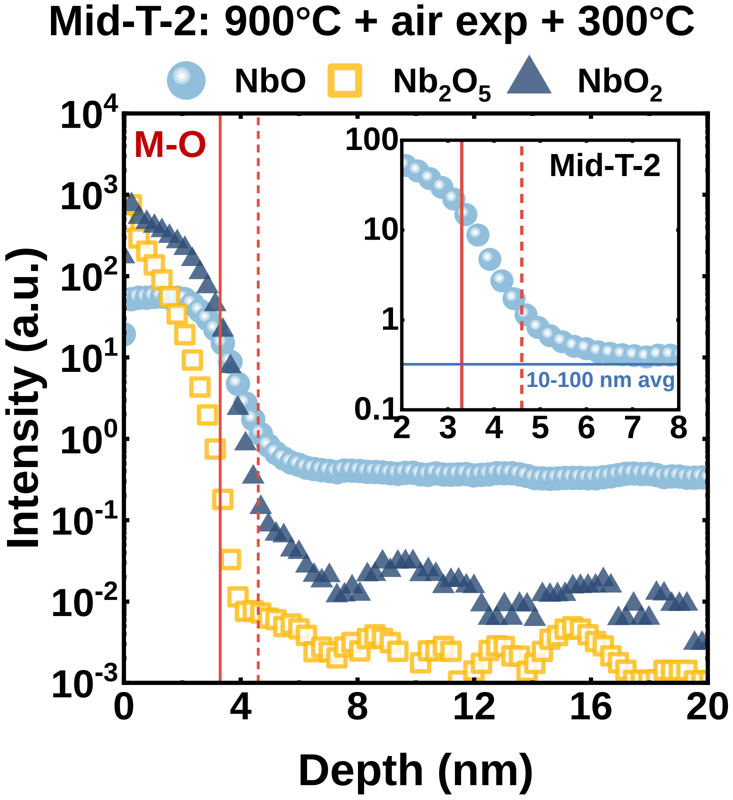




- This oxygen incorporation is beneficial because it tunes the electron mean free path toward an optimal moderate dirty limit, thereby reducing R_{BCS}.
- Different routes to Mid-T baking deliver uniform O diffusions – yet the RF performance slightly differs

Characterization of interface oxides





Near-surface SIMS profile. Intensity normalized by Nb^- ions.

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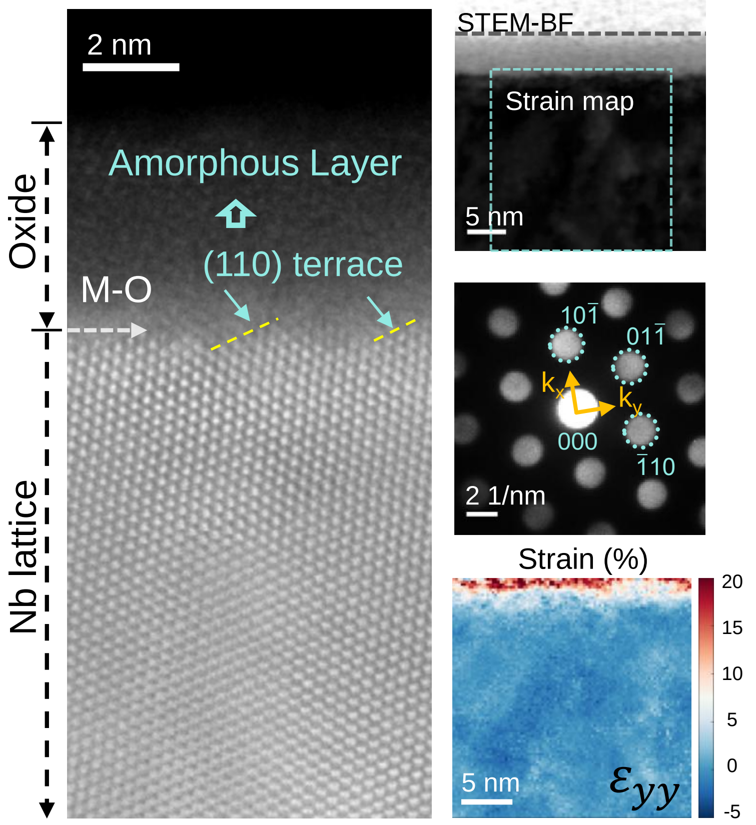
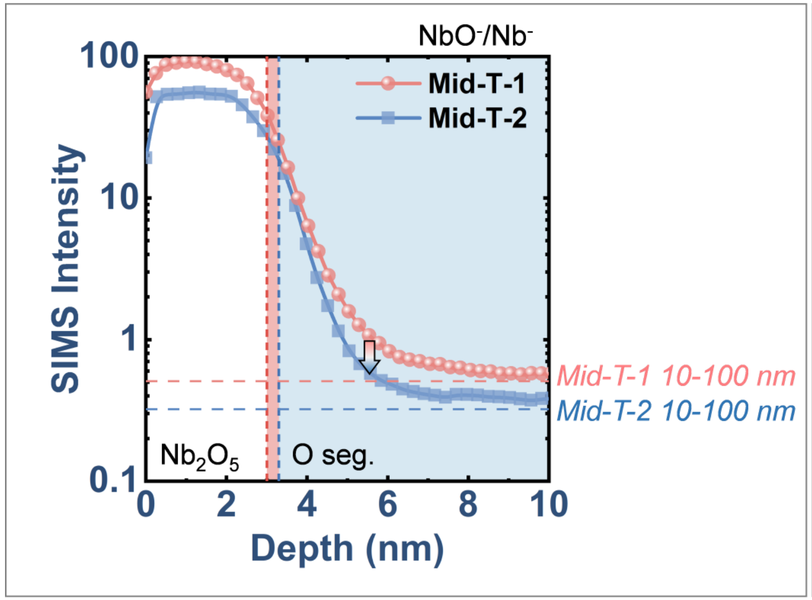


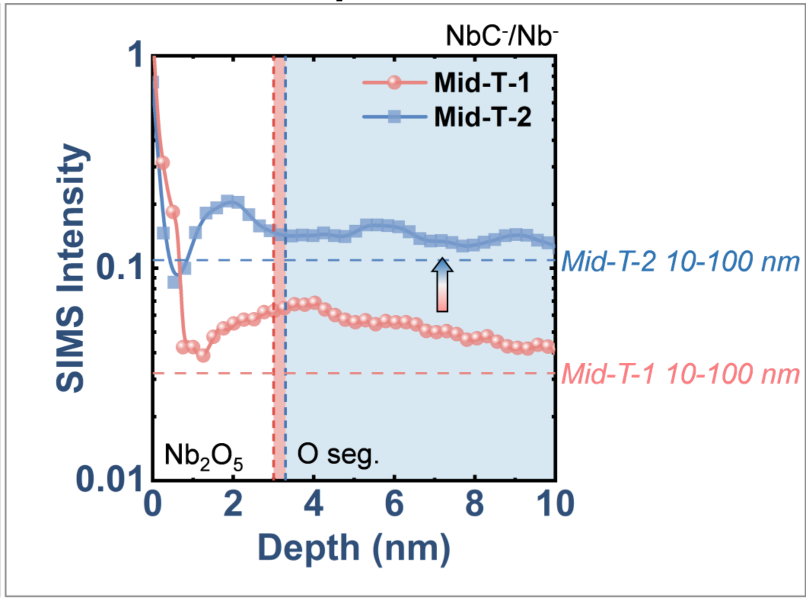
Mid-T-1 produces enhanced oxygen accumulation near the metal–oxide interface. This is associated with higher NbO-related signals and more pronounced lattice disorder and strain.

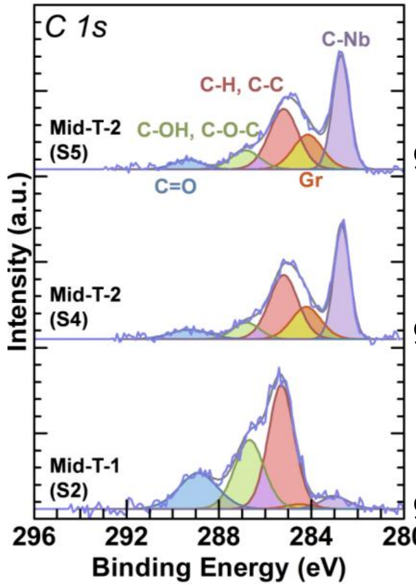
TEM observations of Nb metal-oxide (M-O) interface

The inverse NbC - NbO relationship at M-O interface

Mid-T-1: 900°C + EP + 300°C **Mid-T-2: 900°C + air exp + 300°C**







900°C+Air+300°C

900°C+Air

900°C+EP+300°C

- Mid-T-1: stronger oxygen segregation near the interface.
- Mid-T-2: enhanced carbon/carbide contribution and reduced oxygen segregation.
- Mid-T-2 retains carbide species before/during the 300 °C bake

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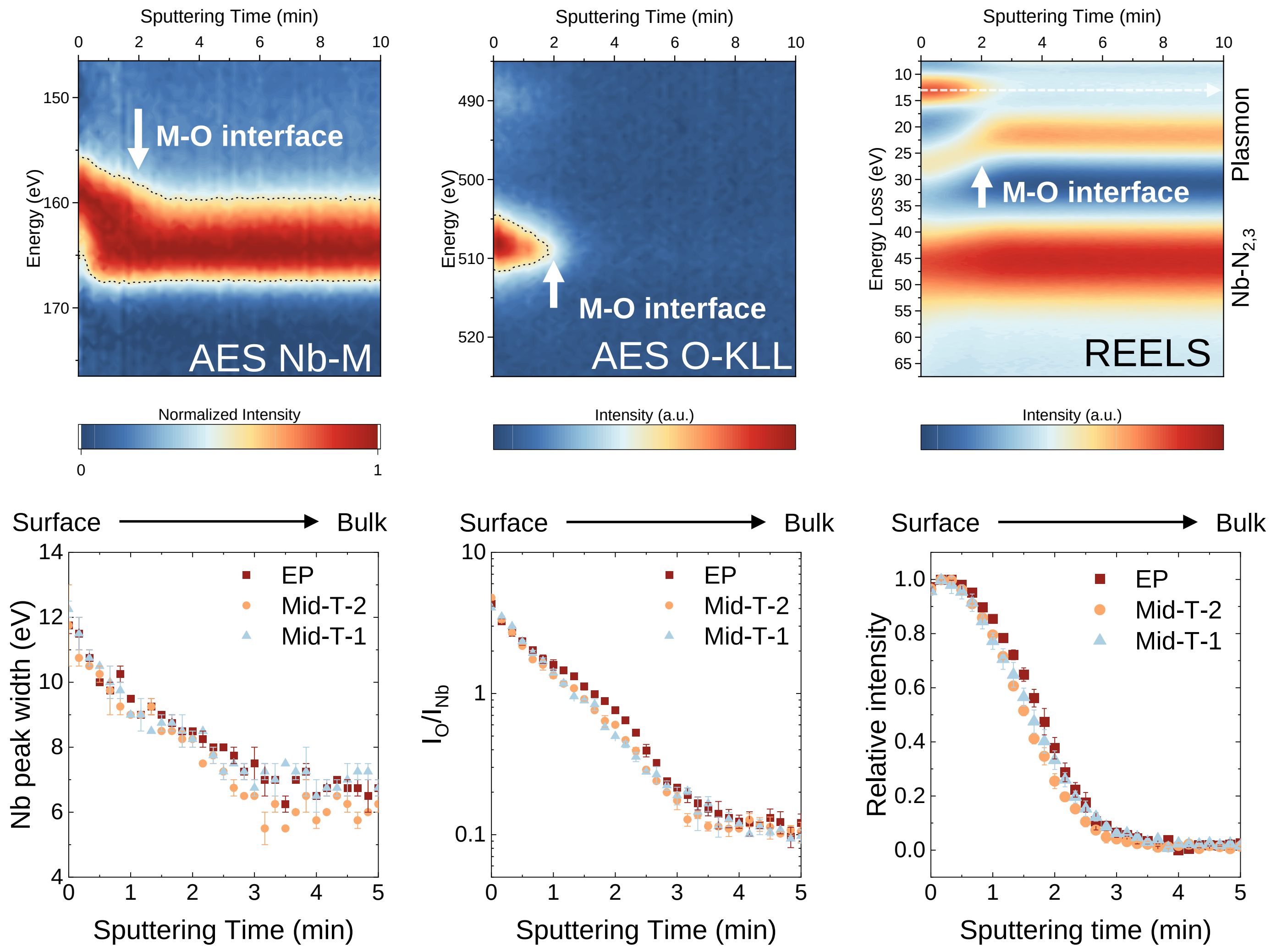
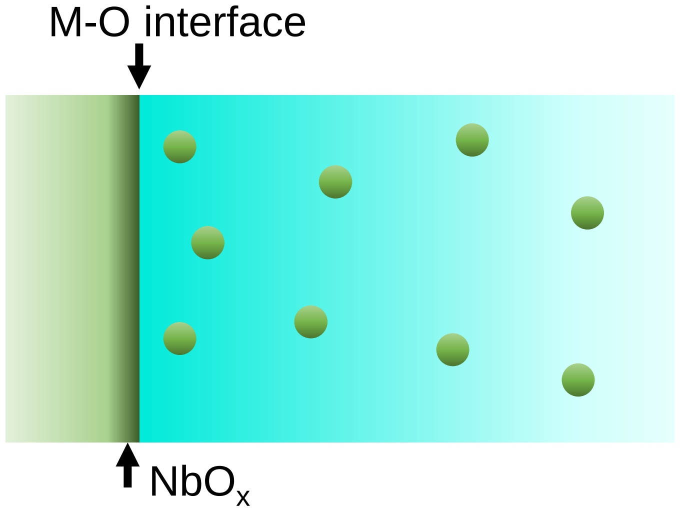
Characterization of interface oxides

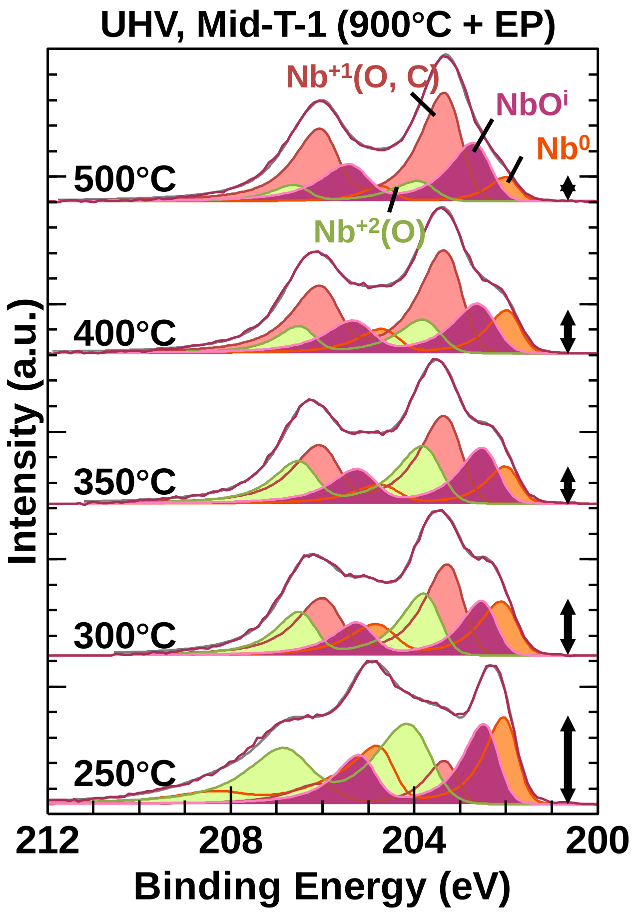


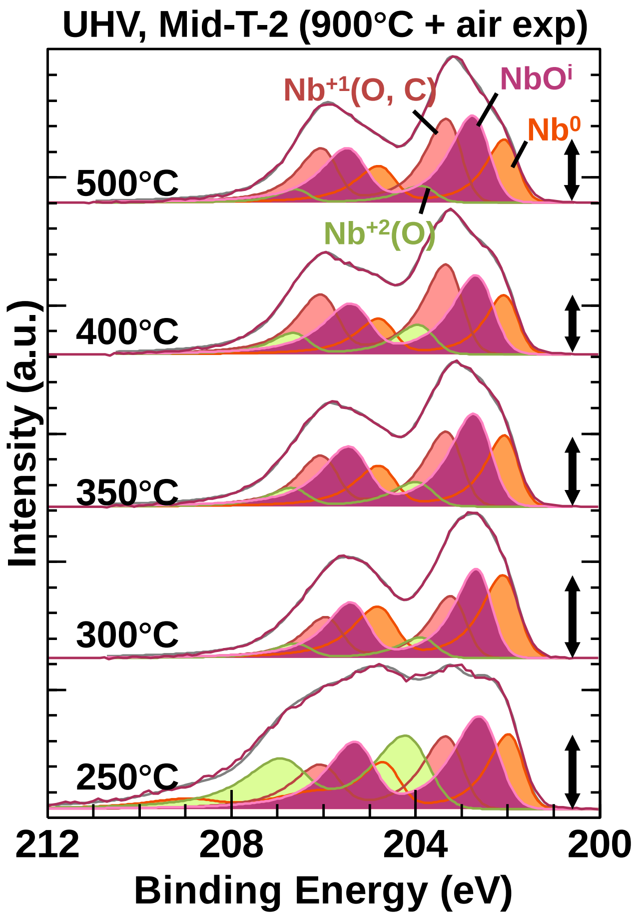


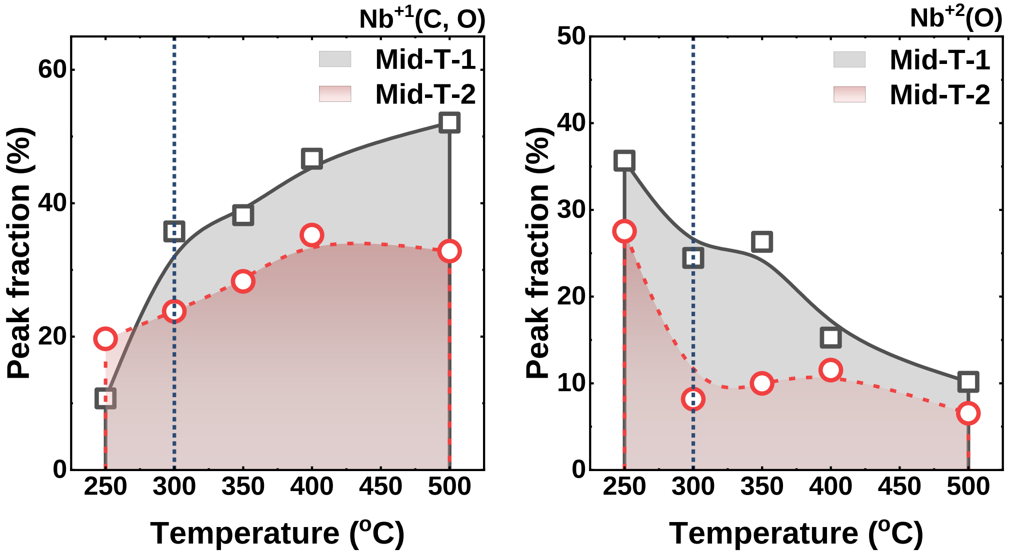
Mid-T-1 retains an EP-like gradual oxide-to-metal transition, implying that the EP-related interfacial legacy is not fully removed by the EP + 300 °C treatment.

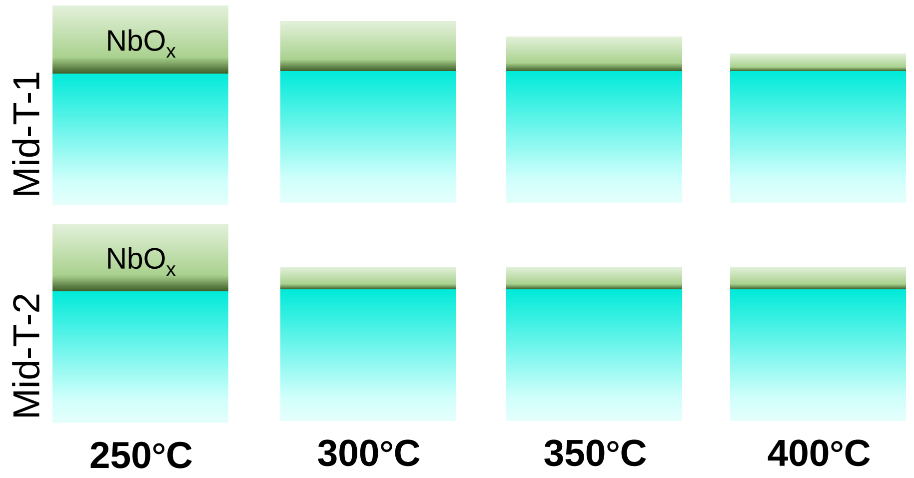
Rate: 1.5 nm/min calibrated against SiO_2

Interface oxides – dissolution behaviors









in-situ XPS spectra of Nb coupons commenced from **900°C + EP** and **900°C + air exposure** processes.

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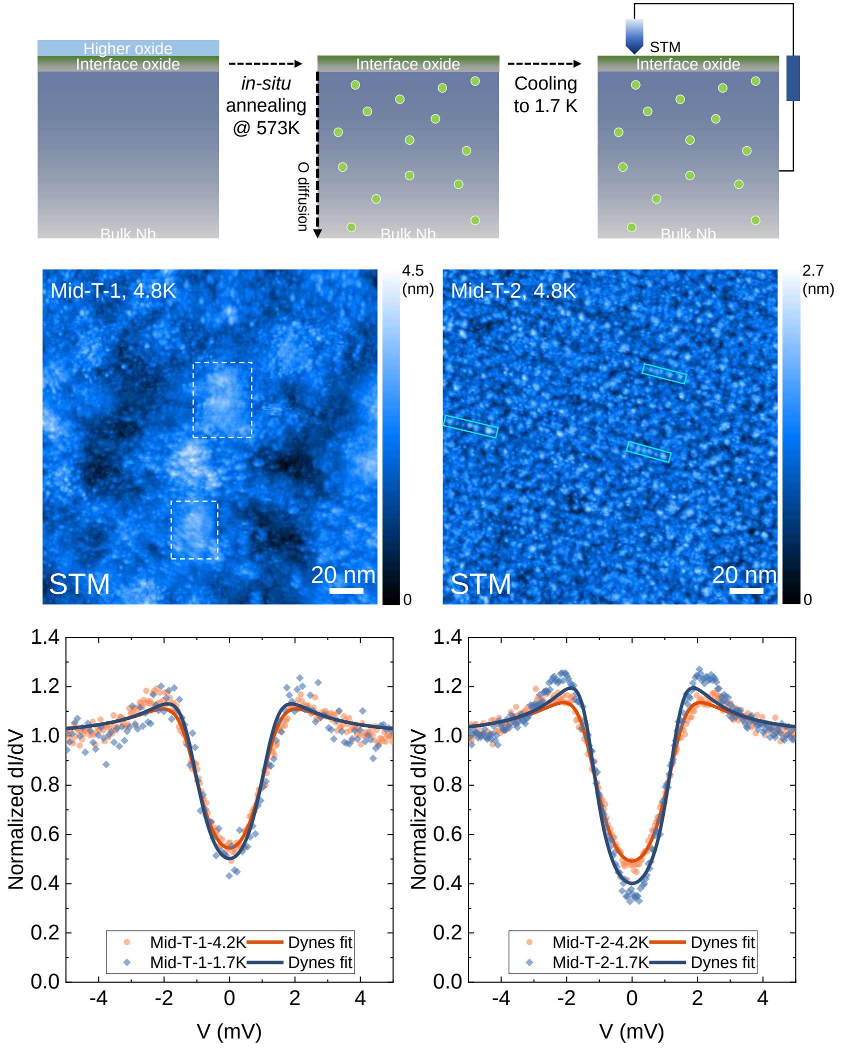
Surface DOS characterizations

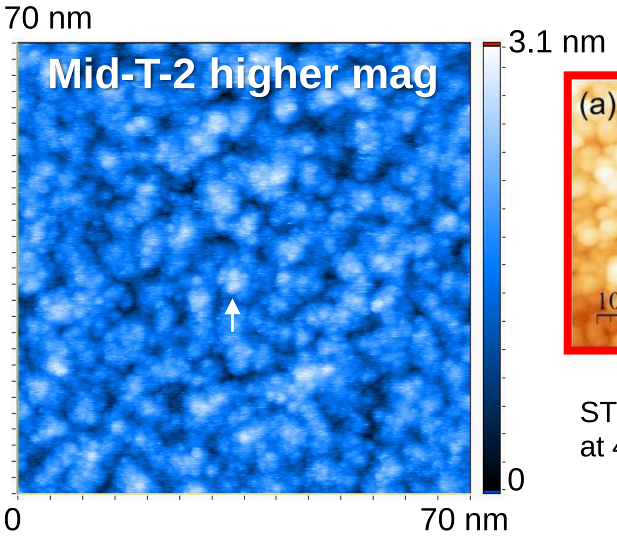


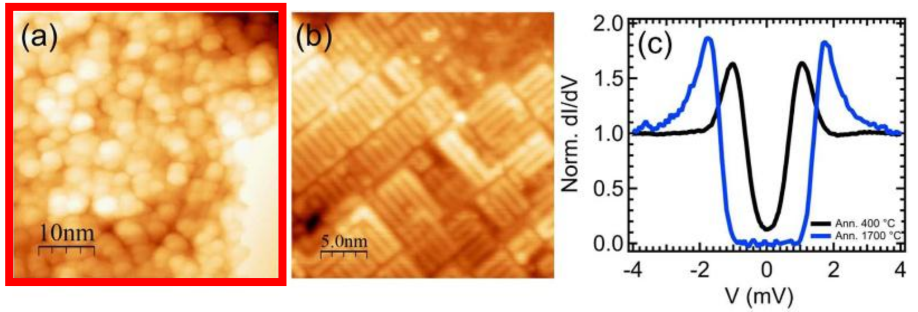
Dynes formula:

$$N(\epsilon) = \mathrm{Re}\frac{N_s(\epsilon + i\Gamma)}{\sqrt{(\epsilon + i\Gamma)^2 - \Delta^2}}$$

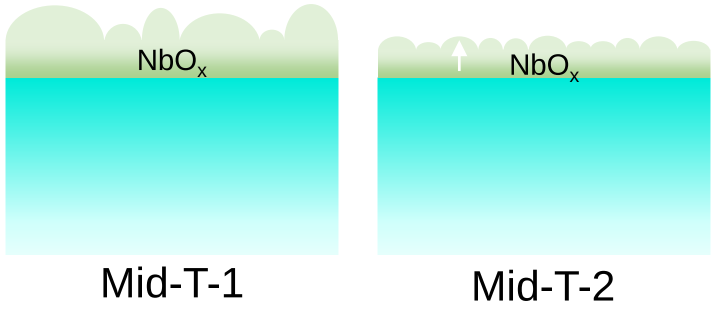
Damping parameter *Γ* quantifies a finite lifetime of quasiparticles ~ *ħ / Γ*.

Finite N(0) at the Fermi level yields residual resistance.

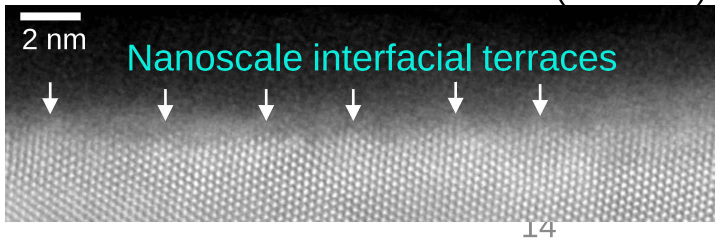




STM topography image of a Nb (100) single crystal after annealing at 400°C and 1700°C. *Supercond. Sci. Technol. 37 (2024) 095006*



STEM (side view)



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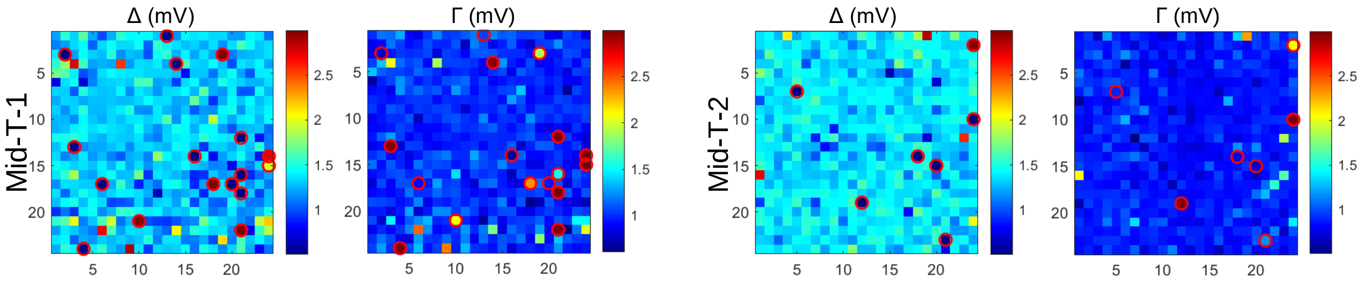
Surface DOS characterizations

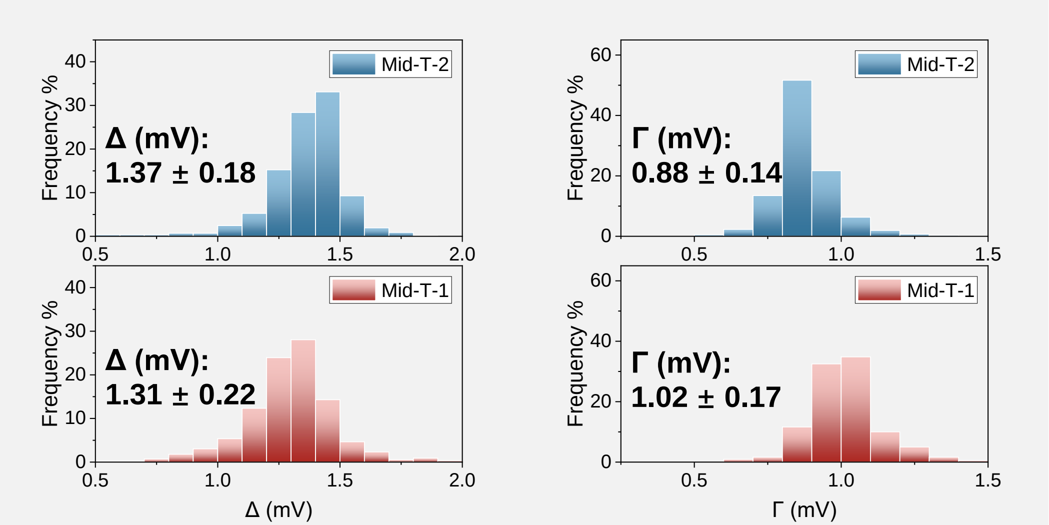
Summarized Dynes parameters from the tunneling spectra measured on *in-situ* annealed specimens. For each condition, the data were collected at ≥ 8 random locations.

Sample ID	Temperature (K)	Δ (mV)	Γ (mV)	Γ/Δ
Mid-T-1	4.9	0.93±0.13	**1.13±0.14**	**1.21±0.09**
	4.2	1.25±0.10	**0.88±0.06**	**0.71±0.08**
	1.7	1.25±0.10	**0.65±0.08**	**0.52±0.10**
Mid-T-2	4.9	**0.96±0.12**	0.81±0.08	0.85±0.06
	4.2	**1.36±0.06**	0.82±0.03	0.60±0.03
	1.7	**1.36±0.06**	0.63±0.05	0.46±0.04



T: 4.2K. Pixel distance: 29.2 nm, Frame size: 700 nm × 700 nm.

- **Mid-T-1**: Large Γ, strong scattering (broadening of the DOS) at the metal surface.
- **Mid-T-2**: Reduced Γ/Δ ratio, uniformly distributed, weakened scattering and prolonged quasiparticle lifetime.
- Impact: Sharper DOS peaks, lower residual Rs.
- (XPS) Thinner interface oxide for Mid-T-2: reducing subgap states, suppressing DOS broadening.
- Lateral uniformity: minimizing "hotspot" dissipation.



Summary and outlook

- This work demonstrates that medium-temperature baking can simultaneously enhance the quality factor Q_0 and the maximum E_{acc} of 1.3 GHz bulk niobium SRF cavities by atomically engineering impurity distributions at the Nb/oxide interface.
  - Mid-T-1 produces a stronger anti-Q slope but tends to show a lower maximum accelerating gradient.
  - Mid-T-2 yields a shallower anti-Q slope but superior high-field performance.

Summary and outlook

- Proposed Mechanism for Simultaneous Q_0 and E_{acc} (max) Enhancement
  - Oxygen doping reduces BCS resistance: Moderate oxygen diffusion into Nb tunes the electron mean free path and reduces R_{BCS}, giving high Q_0 and anti-Q slope behavior.
  - Carbon suppresses NbO segregation: In Mid-T-2, carbon-related species suppress excessive oxygen segregation and NbO formation at the interface.
  - Reduced interfacial disorder improves high-field performance: A cleaner, more homogeneous Nb/oxide interface reduces quasiparticle broadening, subgap states, vortex nucleation probability, local weak superconducting regions, and residual RF losses.
- **Mid-T-2 simultaneously preserves beneficial oxygen doping in the RF penetration layer while suppressing detrimental interfacial oxygen segregation.** This balance explains why Mid-T-2 achieves both high Q_0 and E_{acc} (max) .
- Future perspective:
  - Surface treatments: how to bridge the gap between cavity performances, treatment process, material structures and fundamental theories?

Thank you!

Welcome to visit ShanghaiTech and SHINE.

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