
Atomic Growth Modes of Metal Coatings on Nb for SRF Cavities

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The University of Chicago

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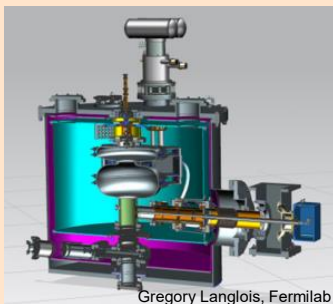
SRF Cavities Efficiently Accelerate Particles



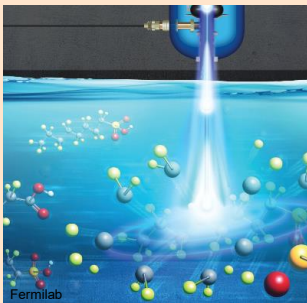
Radio-frequency cavities are the most common and efficient method for accelerating charged particles at high energy.

Applications

Medical Sterilization

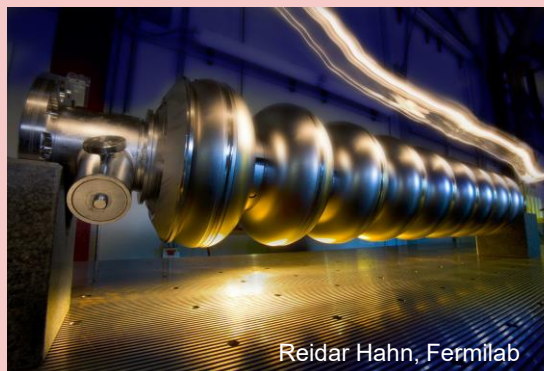


Degradation of PFAS



Current Operation

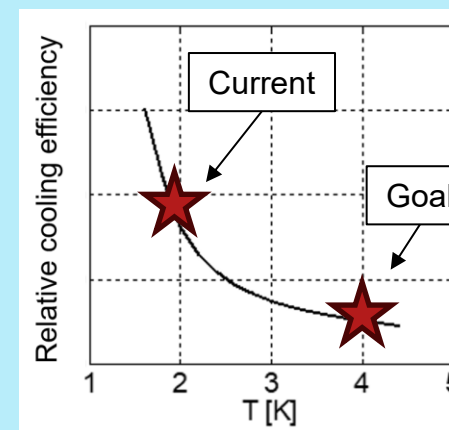
Nb SRF Cavity



- High-purity Nb cavities
- Operate at 2 K
- $Q \approx 10^{10}$

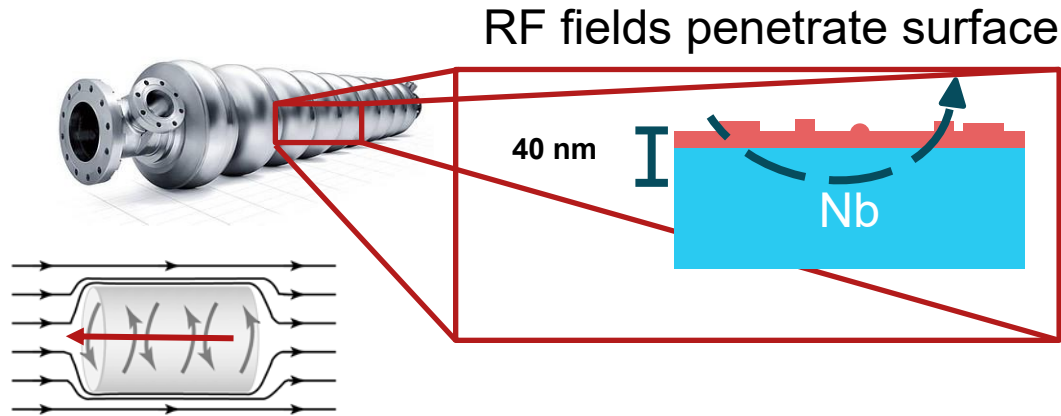
Our Goal

Increase operating temperature while reducing cooling requirements





Why the Surface Matters

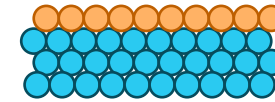
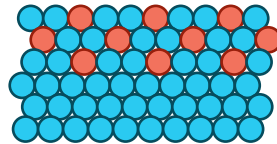


RF fields penetrate only the first ~40 nm of the Nb surface, making this region critical to cavity performance.

Surface Enhancement Strategies at CBB

Alloying Layers (Nb_3Sn , Zr-Nb)

Capping Layers (Au)



Rather than replacing the entire niobium cavity, we focus on engineering only the surface to produce coatings that reduce RF losses and enable higher-performance SRF cavities.

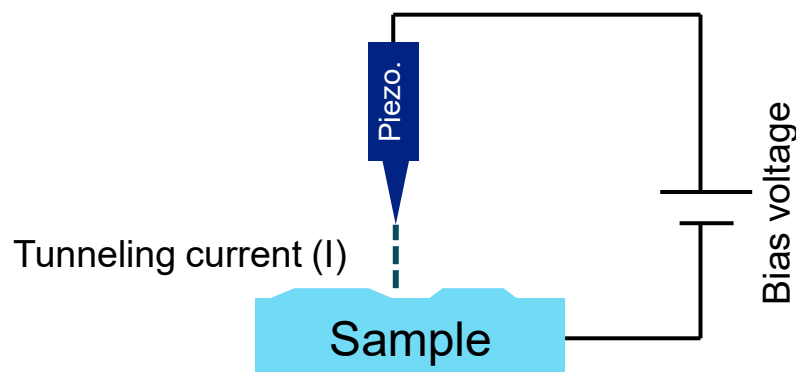


STM Shows Atomic Topography of Coatings



Understanding **how these metal films nucleate and grow** is essential for producing uniform, high-performance coatings.

$$I \propto V \rho_s(E_F) e^{-2\kappa z}$$



- Atomic-scale spatial resolution
- Sensitive **surface topography** and **electronic structure**
- Tunneling current (I) changes exponentially with tip height (z)

STM allows us to observe the **initial nucleation and growth** of metal coatings while simultaneously probing their local electronic properties.

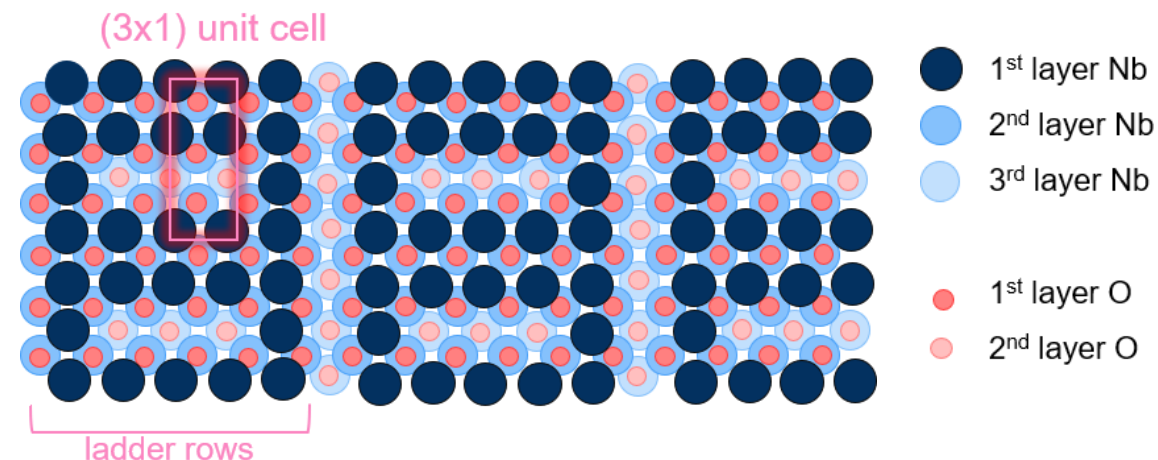


Model System for Rapid Thin-Film Growth Studies



Model system of Nb(100) single crystal

- (3×1) -O/Nb(100) structure (NbO)
 - Highly ordered surface allows visualization of atomic surface changes
- UHV Chamber with STM, PVD, Chemical Analysis (XPS, UPS, AES)





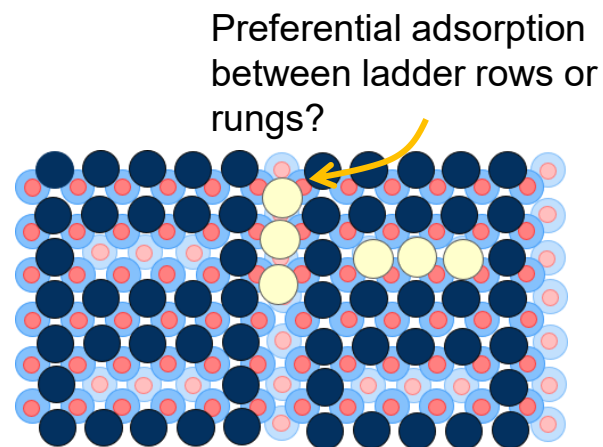
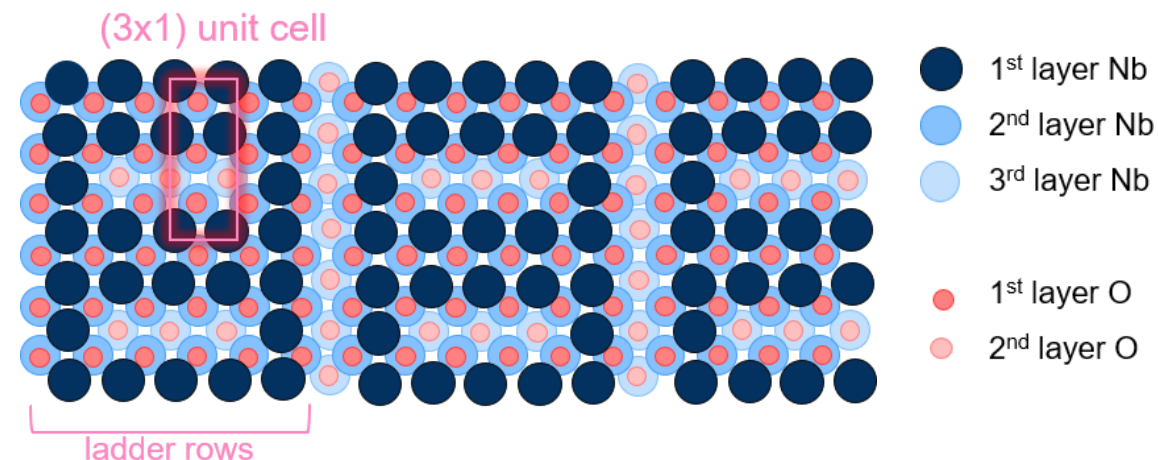
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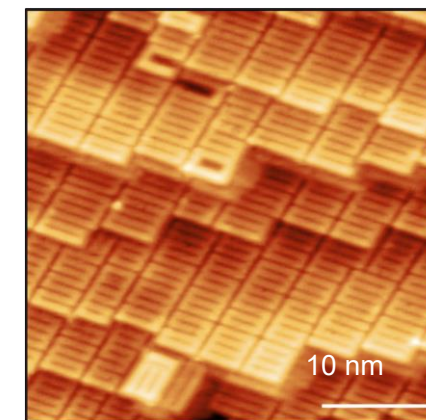
Model system of Nb(100) single crystal

- (3×1) -O/Nb(100) structure (NbO)
 - Highly ordered surface allows visualization of atomic surface changes
- in-situ PVD with STM

The nucleation stage determines the final film morphology and uniformity.



STM of (3×1) -O/Nb(100) structure



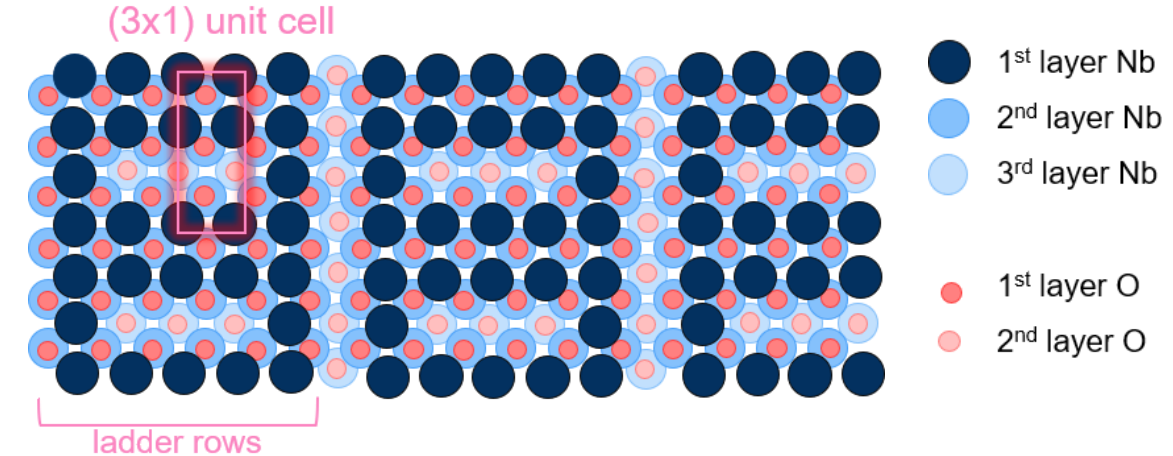


Model System for Rapid Thin-Film Growth Studies



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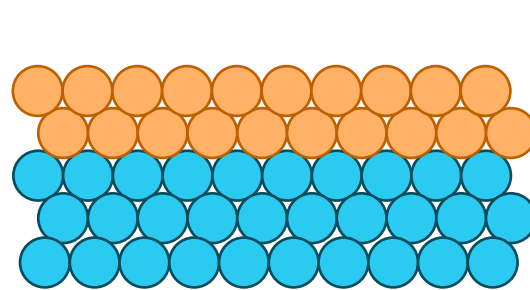
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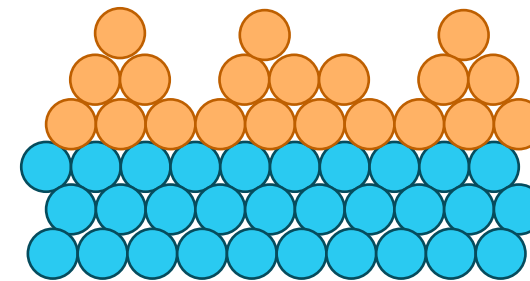
The model system enables systematic studies of nucleation by varying:

- Deposition Rate
- Substrate Temperature
- Surface Preparation

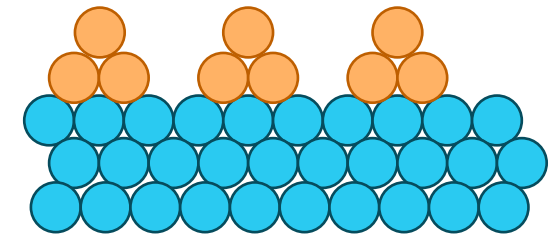
Growth mechanism



Frank-van der Merwe
(Layer-by-Layer)



Stranski-Krastanov
(Layer Plus Island Growth)



Volmer-Weber
(Island Growth)



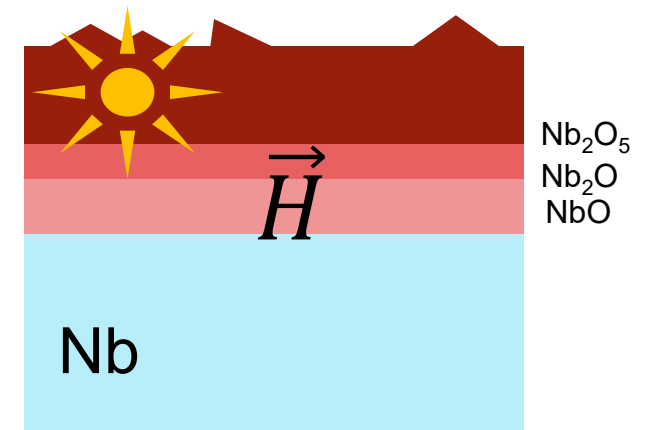
Preventing Lossy Nb Oxide Formation



Nb forms deleterious oxides that limit accelerating performance.

- Nb readily forms insulating oxides that increase RF losses and promote quench
- Native Nb_2O_5 Formation
 - Amorphous
 - Insulating, non-SC
 - 5-7 nm

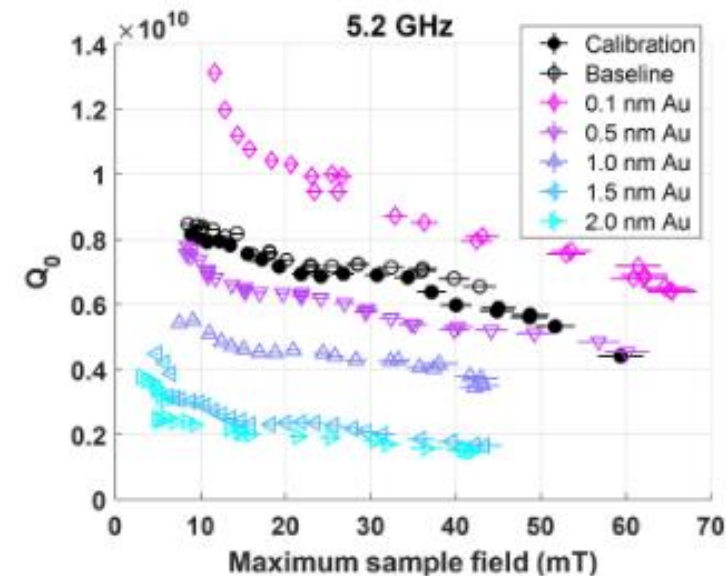
Oxides create localized heating.





Nb forms deleterious oxides that limit accelerating performance.

- Au capping layers have been shown to increase Q-factor
- Caveat! The effectiveness of Au depends on forming a continuous ultrathin film.



Oseroff, T.; Sun, Z.; Liepe, M. U. *Supercond. Sci. Technol.* **2023**, 36 (11), 115009.

An atomic-scale, mechanistic investigation is needed to understand Au nucleation and growth.

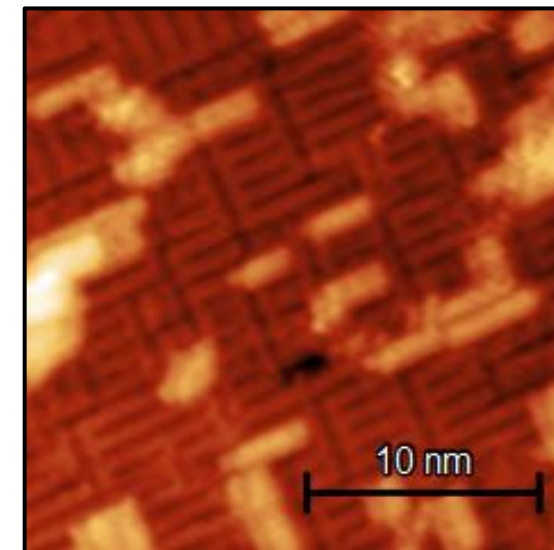
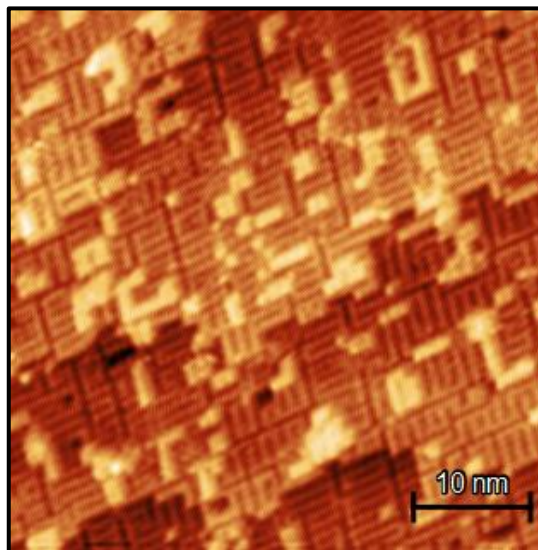


Low Au Coverage Leads to Island Formation



- **0.25 ML Au deposition on $(3 \times 1)\text{-O/Nb(100)}$**
- 10 minute anneals
 - 500°C – Au reorganizes to wire-like island aligned with the $(3 \times 1)\text{-O/Nb(100)}$ reconstruction

500°C



Au nucleates as islands rather than a continuous film.



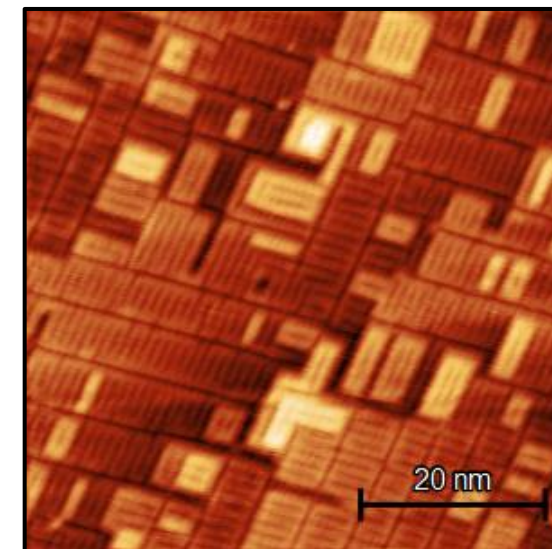
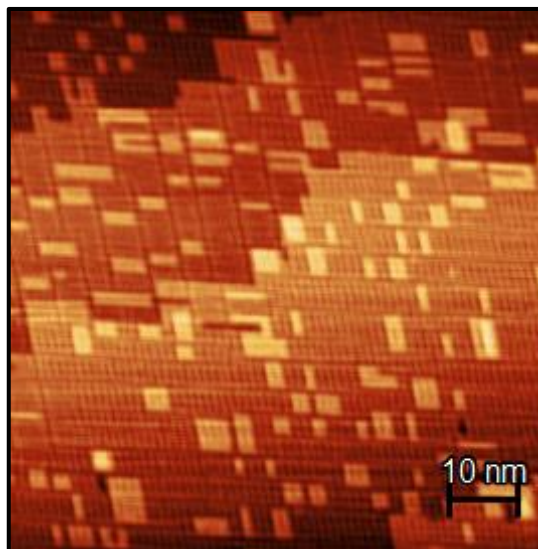
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 - 800°C – Further organization

Annealing enhances ordering but does not produce complete wetting.

800°C



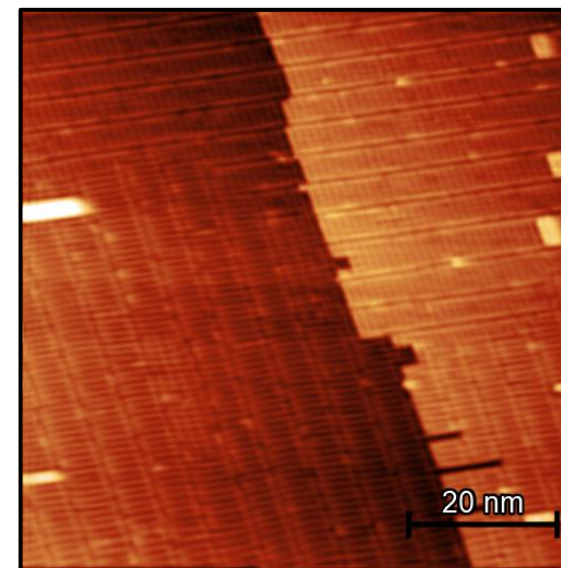


Low Au Coverage Leads to Island Formation

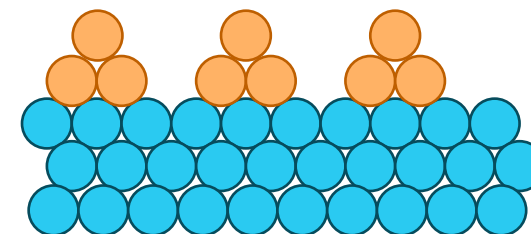


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- 10 minute anneals
 - 500°C – Au reorganizes to wire-like island aligned with the $(3 \times 1)\text{-O/Nb}(100)$ reconstruction
 - 800°C – Further organization
 - 900°C – Au desorption

900°C



Au–Au interactions are stronger than Au–NbO interactions, favoring 3D island formation.



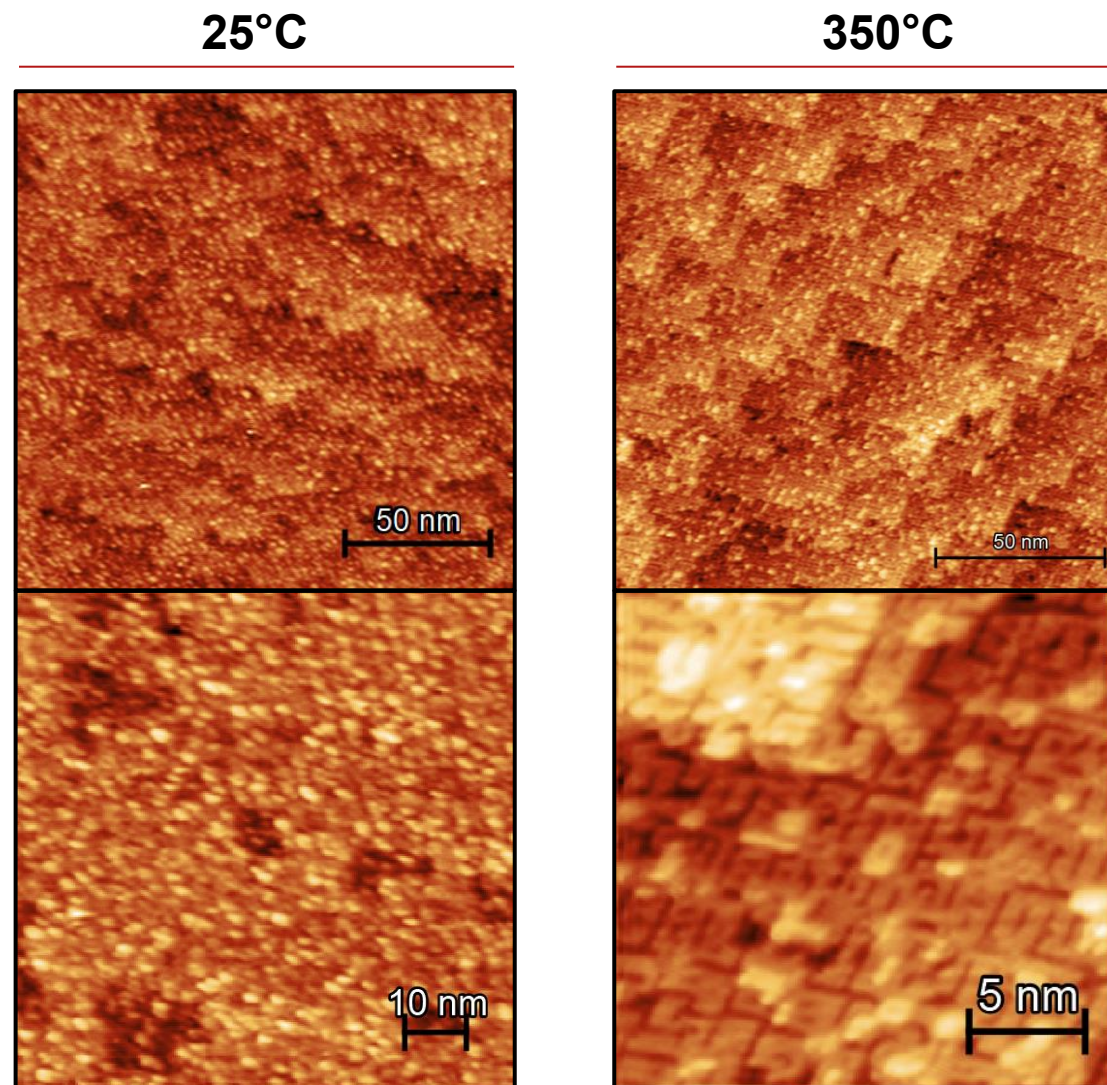


Annealing Promotes to Island Formation



- 1 ML Au deposition on (3×1) -O/Nb(100)
- Post-Deposition (25°C) – Flat but disordered Au coverage
 - 350°C – Au island formation

Although Au initially wets the surface, annealing drives dewetting Au islands, exposing NbO to oxidation.

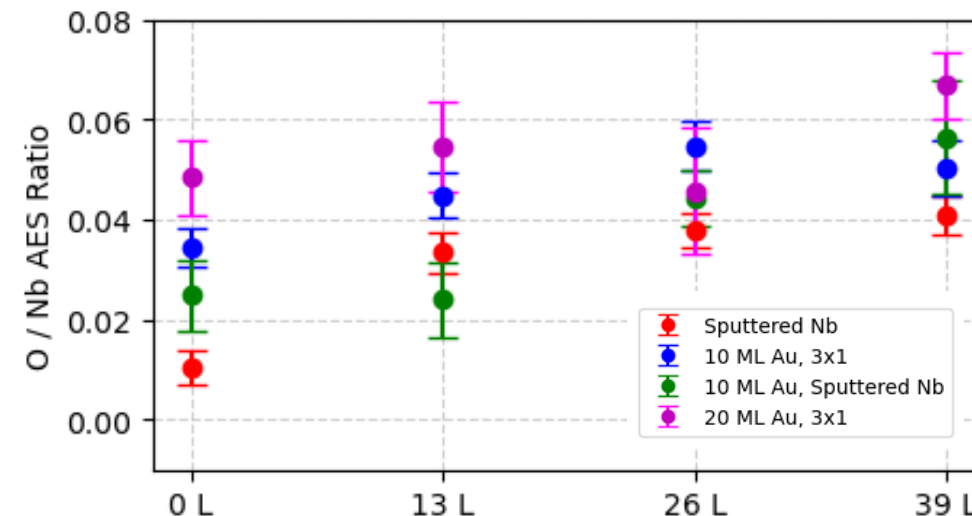




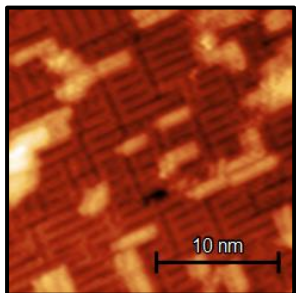
Early Island Nucleation Dictates the Final Porous Morphology Leading to Oxidation



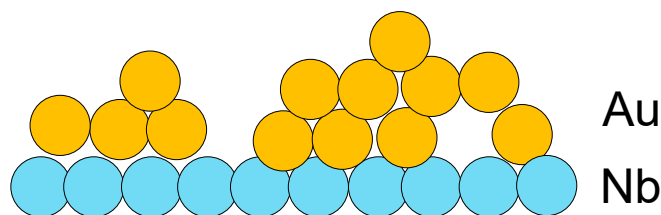
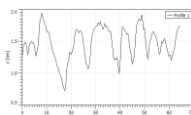
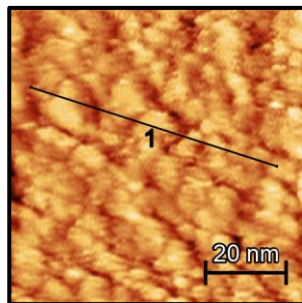
- Au depositions 1-20 ML on
 - $(3 \times 1)\text{-O/Nb}(100)$
 - Sputtered Nb
- Tested anneals from 360°C - 1100°C
- Nb_2O_5 forms after every ATM exposure



STM of 0.25 ML Au on $(3 \times 1)\text{-O/Nb}(100) + 500^\circ\text{C}$



STM of 10 ML Au on $(3 \times 1)\text{-O/Nb}(100) + 800^\circ\text{C}$ Flash



Island formation $\rightarrow$ porous Au layers

Early-stage island nucleation persists during growth, producing porous Au films even at high coverage.

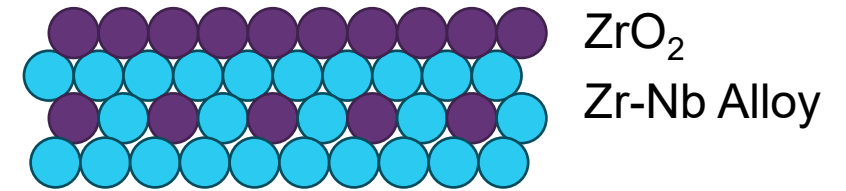


Zr as a Sacrificial Oxygen Getter



Implementation of Zr - Beneficial reactivity

- Zr interdiffusion forms high TC superconducting Nb/Zr alloy (17.7 K)
- Preferential oxidation in Zr/Nb multilayer systems





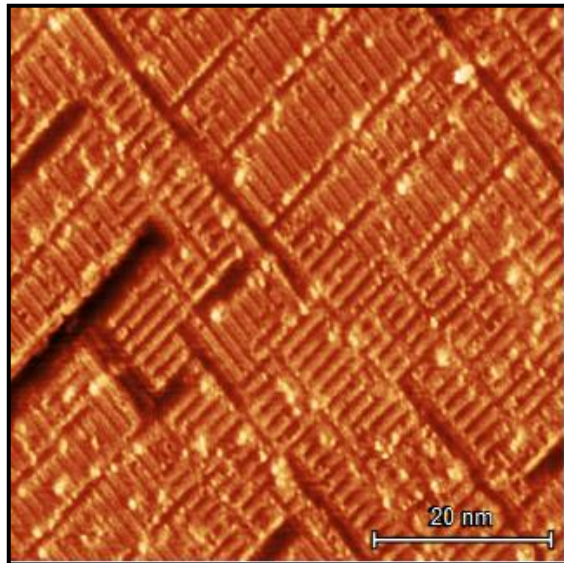
Volmer-Weber Growth of Zr on (3x1)-O/Nb(100)

Initial Zr deposition follows a Volmer–Weber growth mode, producing non-uniform islands rather than atomically flat films.



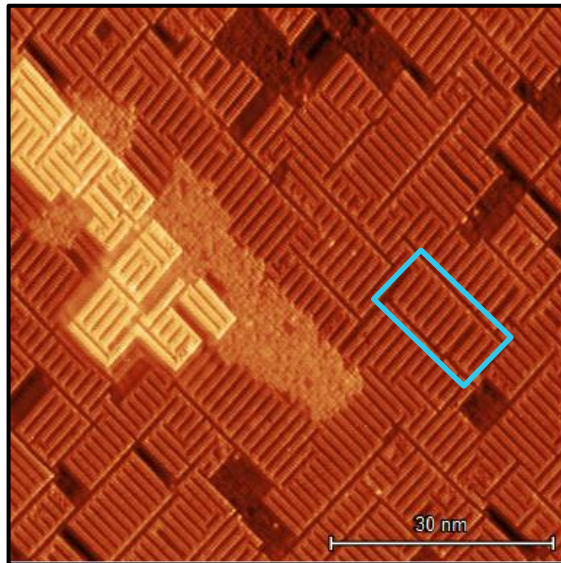
The reconstruction changes from (3×1) to cubic following Zr deposition, suggesting oxygen transfer from NbO to Zr.

Post Deposition at 25 ° C



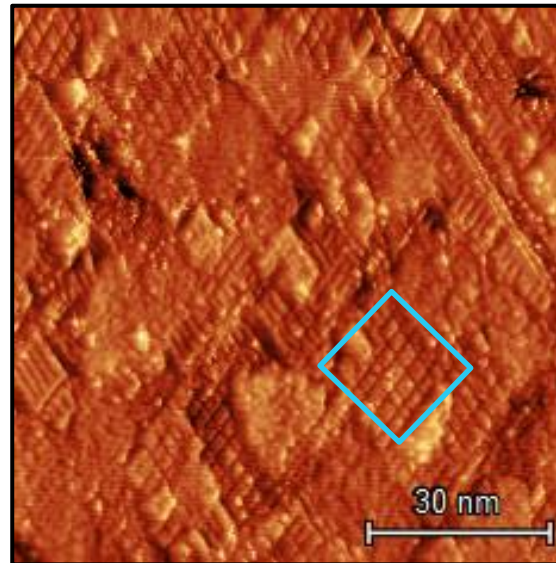
0.15 ML

800 ° C



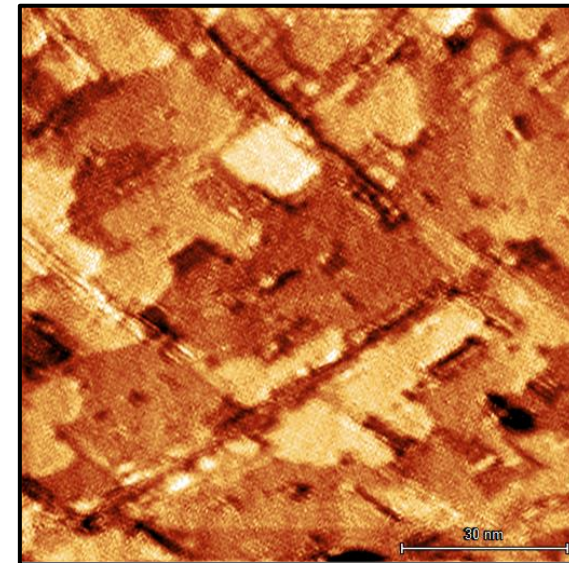
0.15 ML

650 ° C



0.70 ML

650 ° C



0.95 ML



STM Reveals Atomic-Scale Growth of Candidate SRF coatings



- **Au nucleates via Volmer–Weber island growth, producing porous films after annealing.**
- Porous Au coatings expose Nb to oxidation, limiting their effectiveness as protective layers.
- Zr growth also follows Volmer-Weber growth, but **Zr exhibits reactive growth behavior consistent with oxygen scavenging.**

Understanding nucleation and growth provides a pathway toward designing uniform, next-generation SRF material.



Thank you for listening!



Acknowledgements

- CBB
- Sibener Group

