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SRF 2023 GRAND RAPIDS

DESY.

Vacancy dynamics in niobium and its native oxides and their potential implications for quantum computing and superconducting accelerators

Marc Wenskat - on behalf of the SRF R&D Team

at the 2023 International Conference on RF Superconductivity

PHYSICAL REVIEW B **106**, 094516 (2022)

Vacancy dynamics in niobium and its native oxides and their potential implications for quantum computing and superconducting accelerators

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How does mid-T heat treatment affect native oxide…
…and how this correlates with RF performance

Mid-T heat treatment reduces pentoxide thickness

[Rezvan Ghanbari, TTC Workshop, Aomori 2022]

Mid-T heat treatment reduces pentoxide thickness

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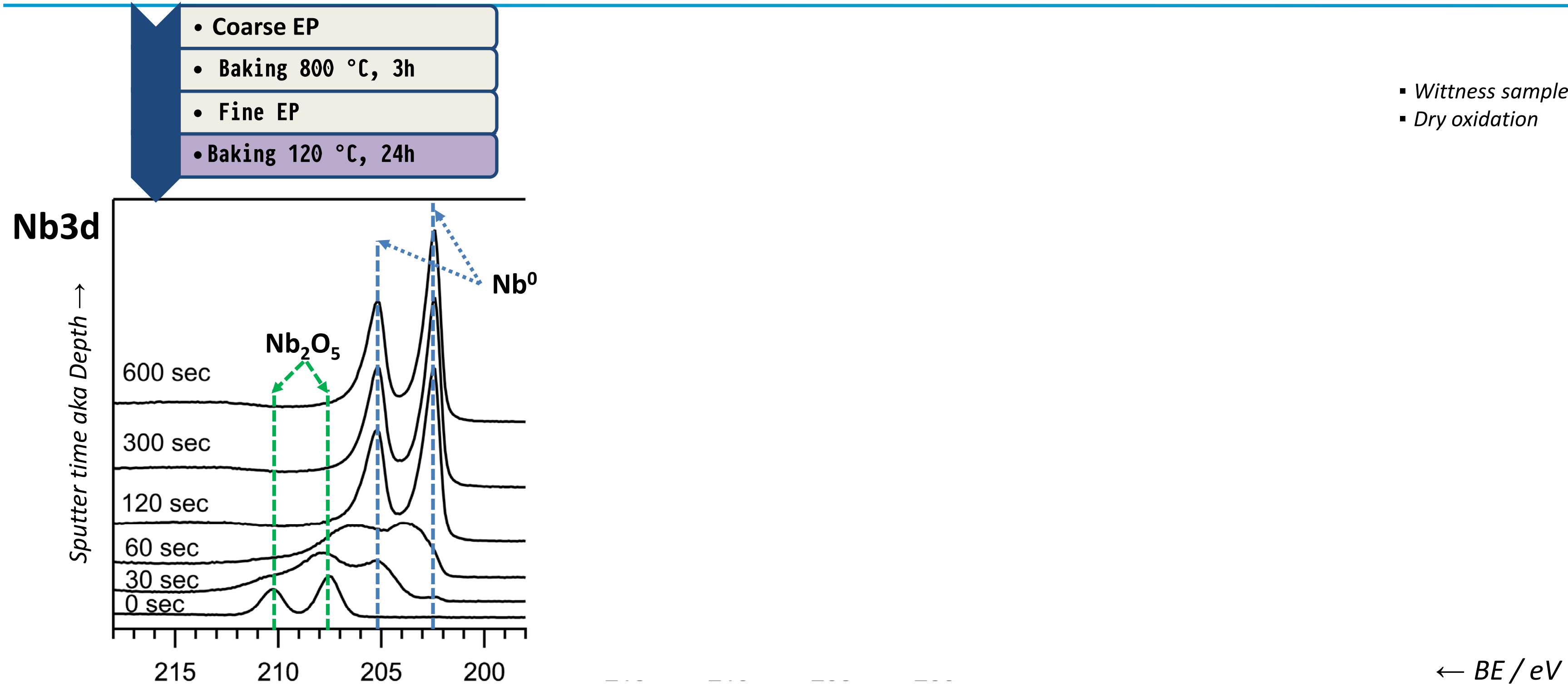
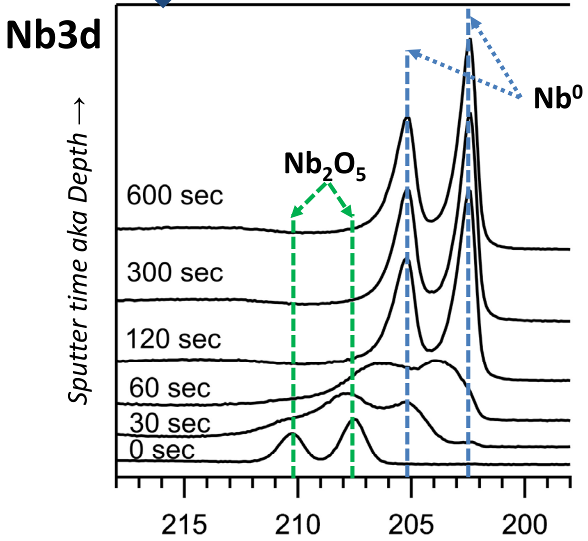


- *Wittness samples*
- *Dry oxidation*

Mid-T heat treatment reduces pentoxide thickness

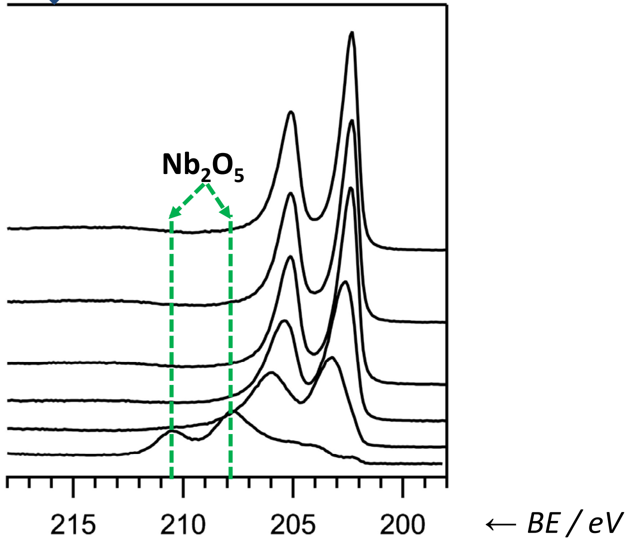
[Rezvan Ghanbari, TTC Workshop, Aomori 2022]

- Coarse EP
- Baking 800 °C, 3h
- Fine EP
- Baking 120 °C, 24h



- Coarse EP
- Baking 800 °C, 3h
- Fine EP
- Baking 300 °C, 3h

- *Wittness samples*
- *Dry oxidation*



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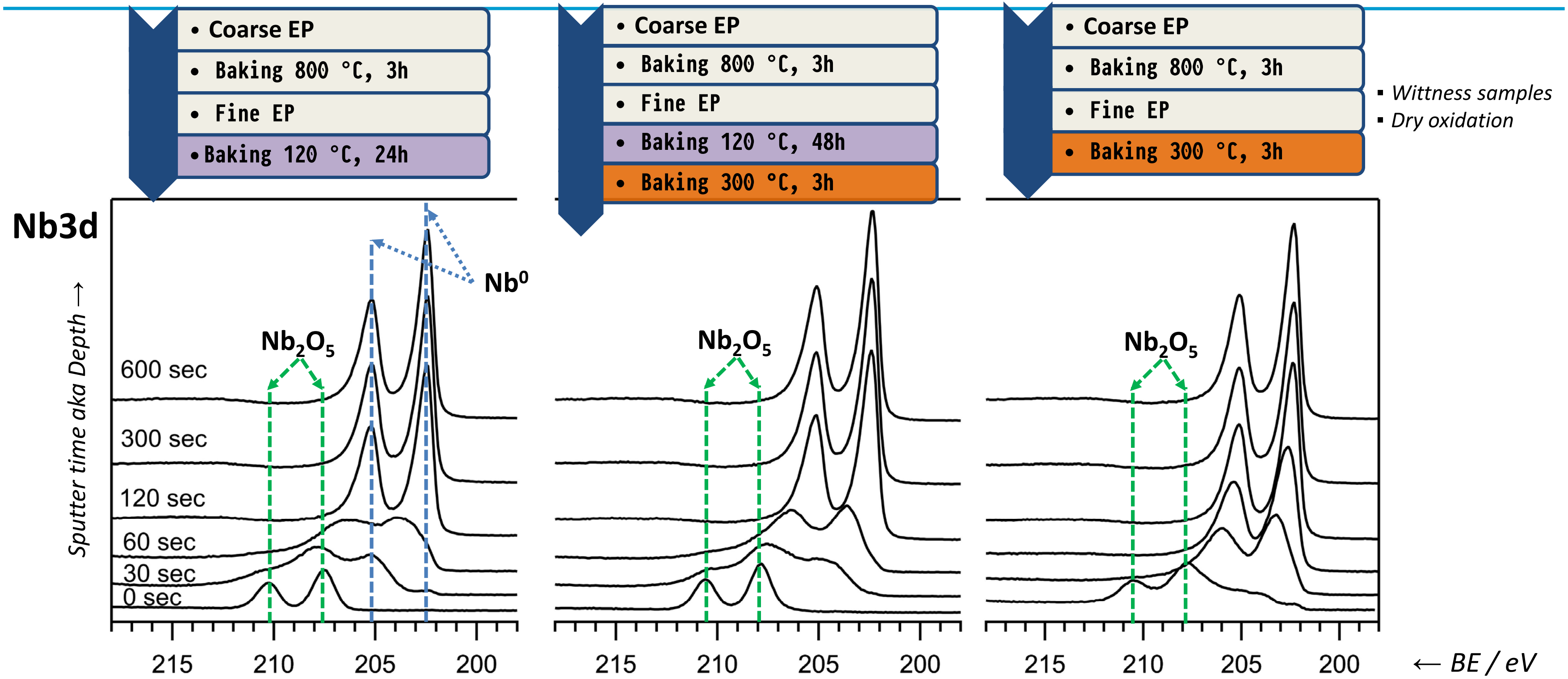
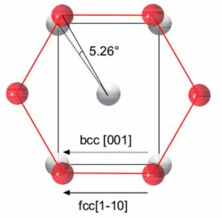


Mid-T heat treatment changes the interface

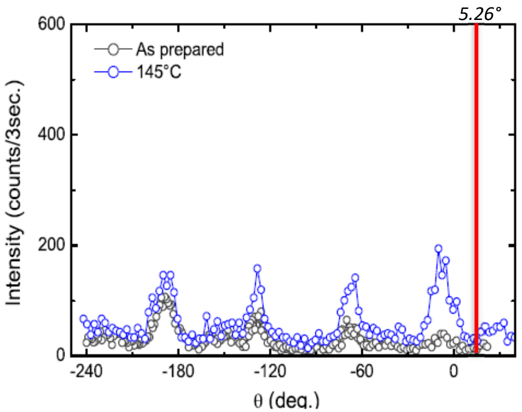
- *Nb – NbO have a lattice mismatch (bcc – fcc) when stacking*
- *For energetic minimum, e.g. for Nb(100), a tilt between cells of 5.26° is expected*
- *In reality, depends on: layer thickness, lattice orientation, growth temperature, interstitial concentration & type*

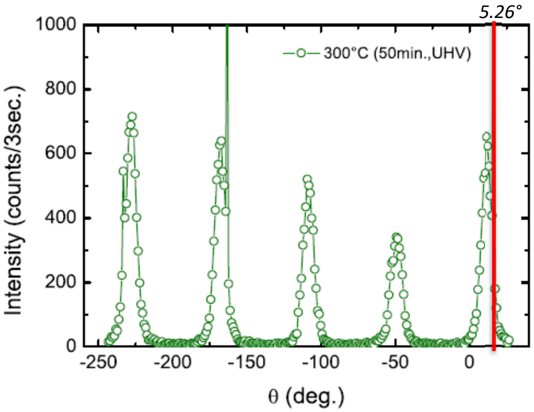
[Zhussupbekov, K., et al. *SciRep* 10.1 (2020): 1-9.]
[Todorova, M., et al. *PRL* 89.9 (2002): 096103.]

Only Nb-atoms shown



Nishiyama-Wasserman (NW)





[Delheusy, M., "X-ray investigation of Nb/O interfaces." Thesis, (2008).]

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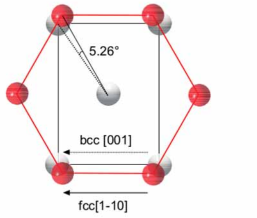

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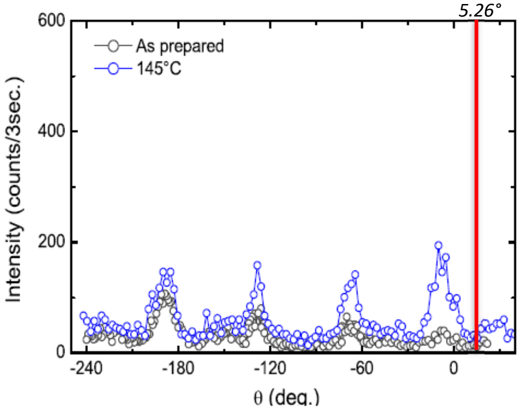
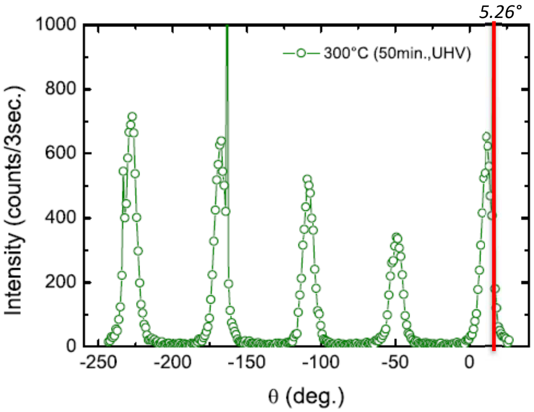
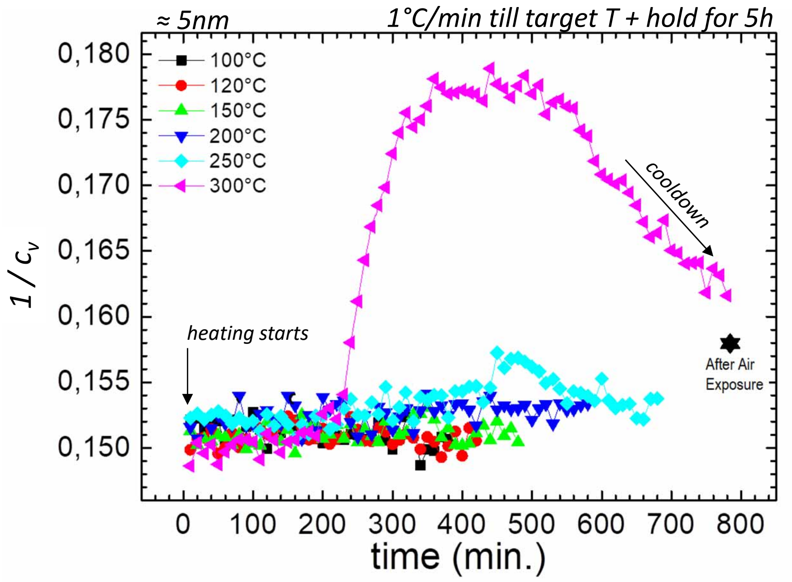




- *In-situ XPS shows a reorganization in the range of 100 – 150 °C*
- *Does the 120°C bake seed a reorganization mitigating the positive effect of the 300°C?*

[Delheusy, M., "X-ray investigation of Nb/O interfaces." Thesis, (2008).]

Mid-T heat treatment reduces vacancy density c_v



- *At 300°C, vacancy density c_v decreases*
- *Remains elevated at RT & even after air exposure!*

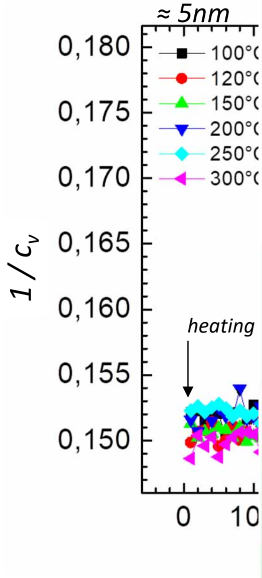
- *O-vacancy in pentoxide create dangling bonds*
  → act as both: magnetic impurities & two-level systems

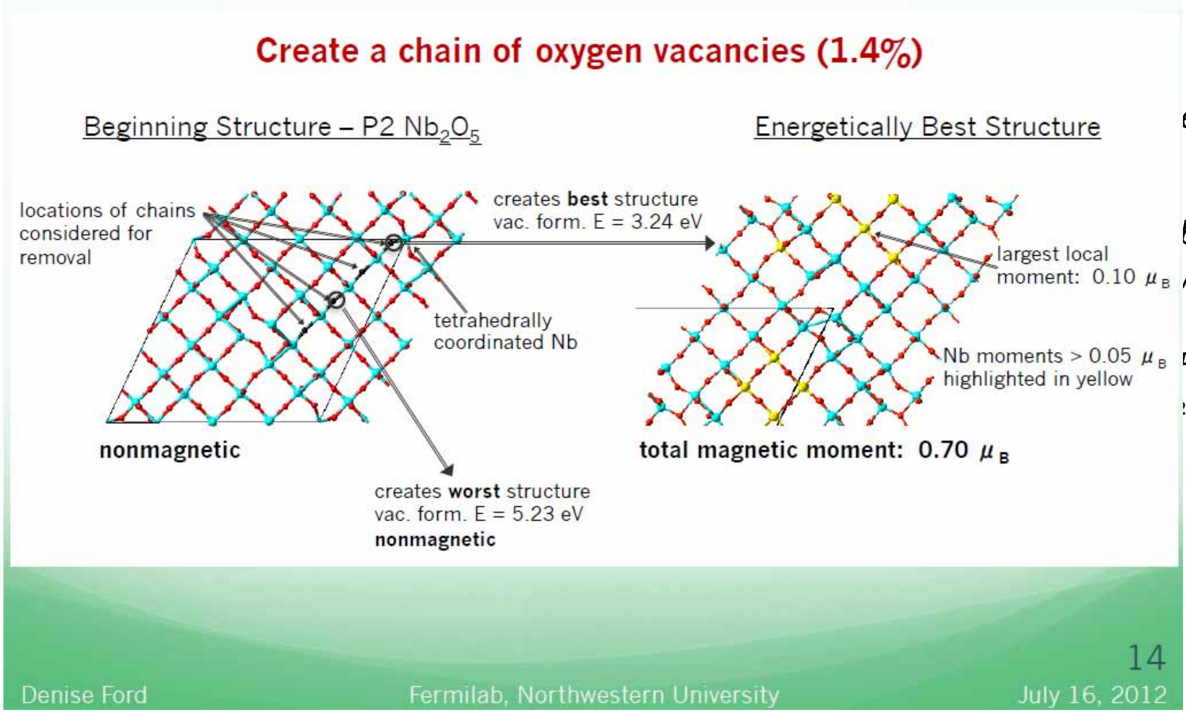
- *Correlation of magnetic impurities and R_s was already shown* **[Proslier, T., et al. *IEEE Trans. Appl. Supercond* 21.3 (2011): 2619-2622.]**

[Wenskat, M., et al., SRF'21 (2021)]

[Wenskat, M., et al., PRB 106.9: 094516 (2022)]

Mid-T heat treatment reduces vacancy density c_v





exposure!

bonds

wo-level systems

R_s was already

2011): 2619-2622.]

[Wenskat, M., et al., SRF'21 (2021)

[Wenskat, M., et al., PRB 106.9: 09

Mid-T heat treatment reduces vacancy density c_v

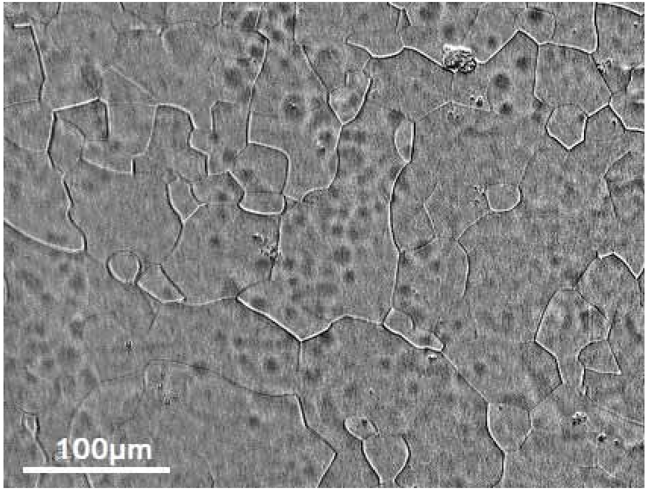
Existence of O-vacancies should lead to surface magnetism – even in the dielectric Nb_2O_5

[Weissmann, M., et al., *Physica B: Condens* 398.2 (2007): 179-183.]
[Venkatesan, M., et al. *Nature* 430.7000 (2004): 630-630.]
[Hong, N.H., et al. *Phys. Rev. B* 73.13 (2006): 132404.]

Oxide layer shows surface magnetism

[Wenskat, M., et al., PRB 106.9: 094516 (2022)]
[Rezvan Ghanbari, TTC Workshop, Aomori 2022]

Magneto-optical image with Kerr microscope



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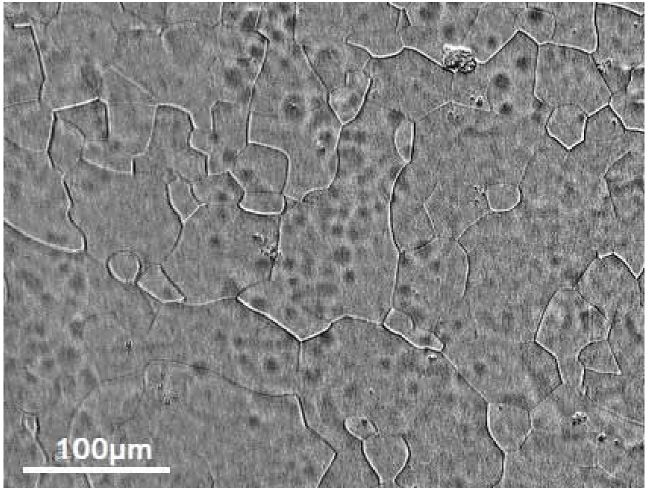

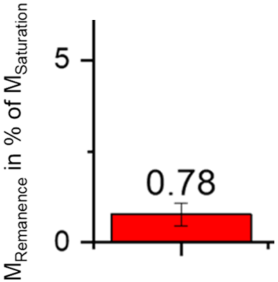

- *120°C baking (Reference)*

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[Rezvan Ghanbari, TTC Workshop, Aomori 2022]

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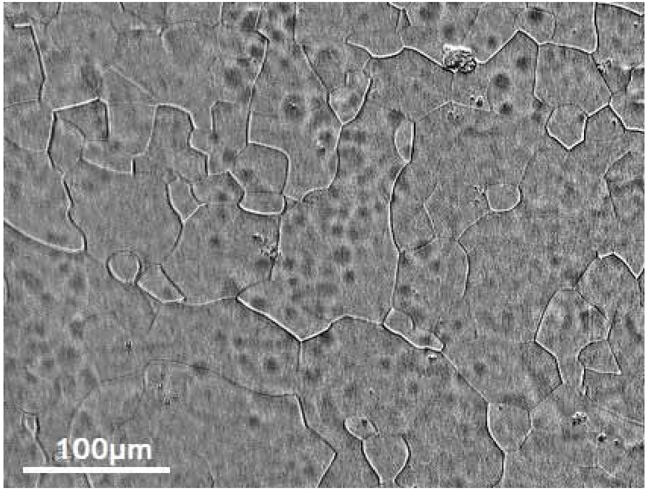

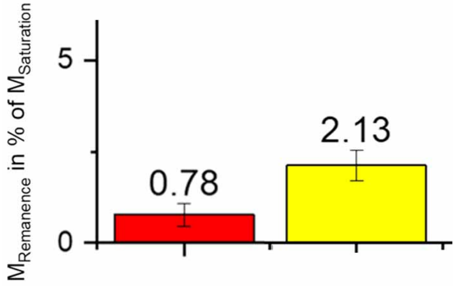

- *120°C baking (Reference)*
- *Accidental baking at p=10^{-4} mbar and 800°C*
  - ➢ *Known from literature: pentoxide grows instead of dissolving*

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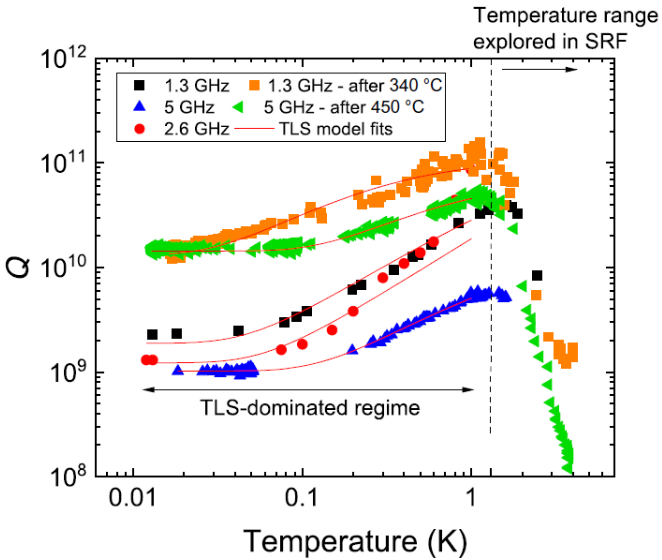
How does this relate to quantum computing R&D?

Two-level-system dissipation describes Q(T) well

[Romanenko, A., et al., *Phys. Rev. Applied* 13, 034032 (2020)]

No oxide: lowest losses



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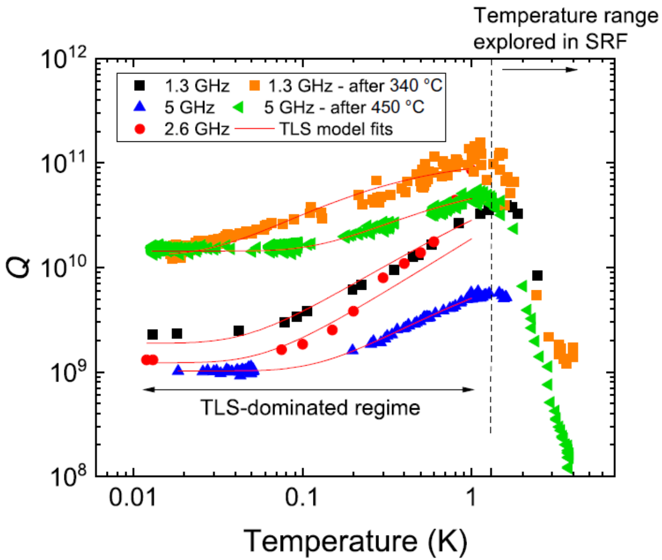
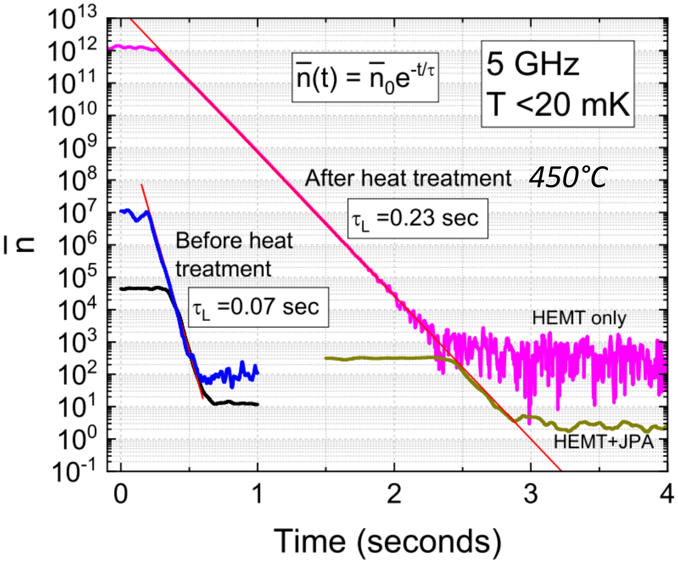


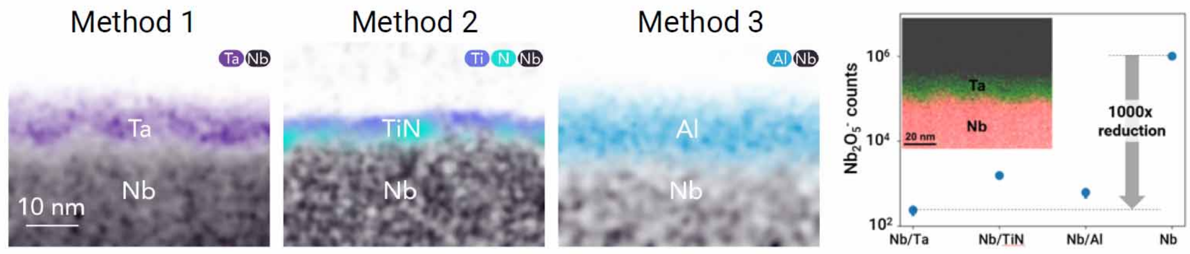
Lifetime improves by the in situ heat treatments at 340-450°C



Encapsulating Nb based qubit improves coherence

[Bal, Mustafa, et al., *arXiv preprint arXiv:2304.13257* (2023)]

Murthy – **TUPTB012**



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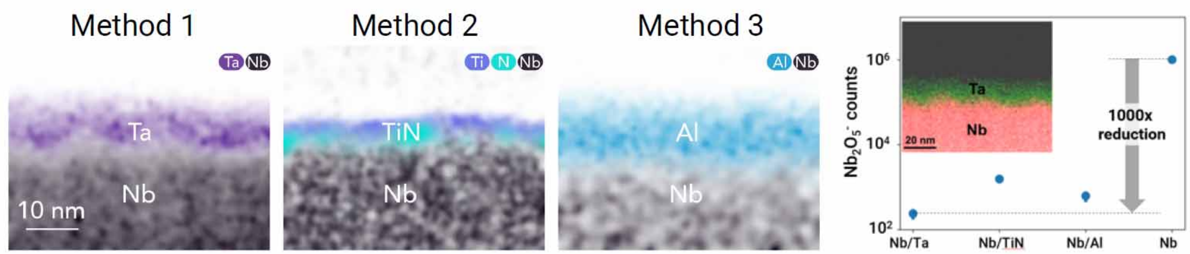
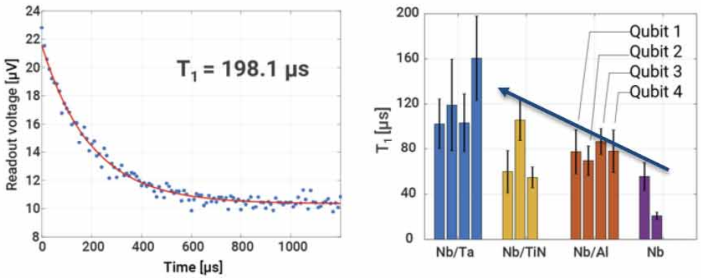


FNAL:



T_1 improved by 3-5x

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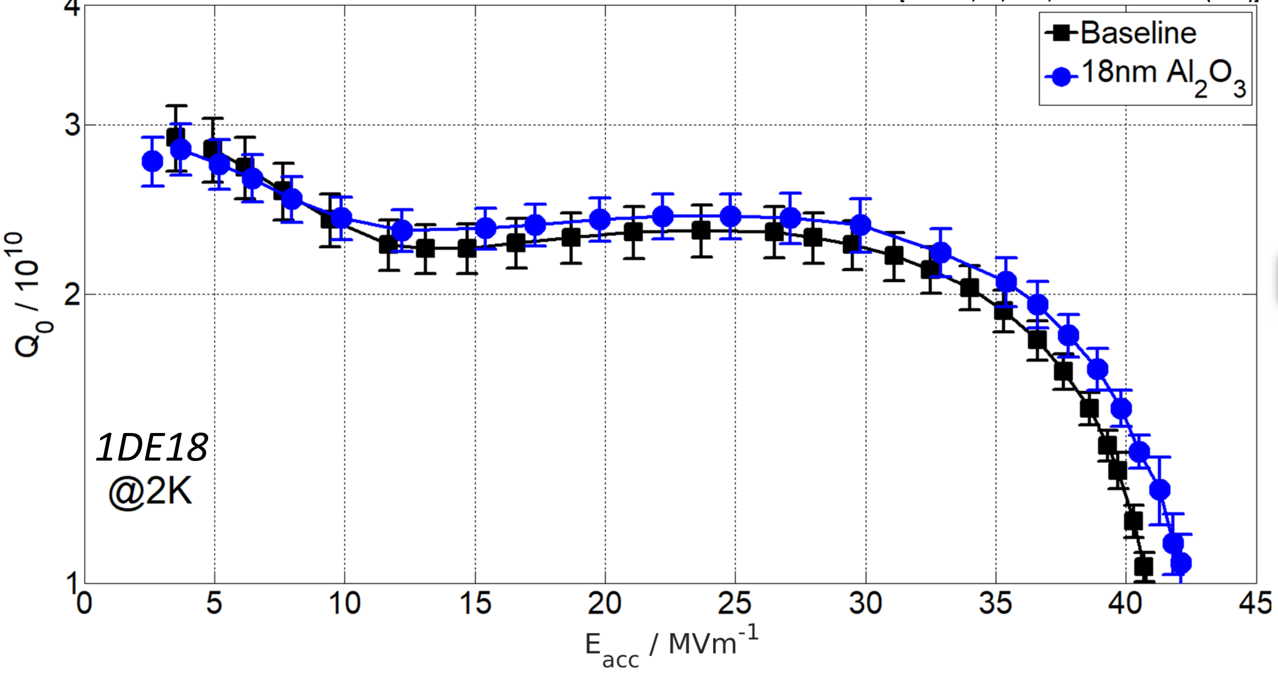
What happens if you test a cavity where the native oxide is replaced?

„Encapsulating“ a cavity with Al_2O_3 via ALD

[Wenskat, M., et al., SUST 36.1 : 015010 (2022)]

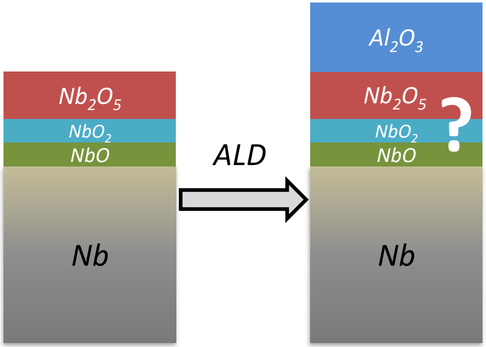


Deyu - **MOPMB016**

González Díaz-Palacio - **WECBA01**

How does the oxide layer evolve?

Zaidmann - **WEPWB072**



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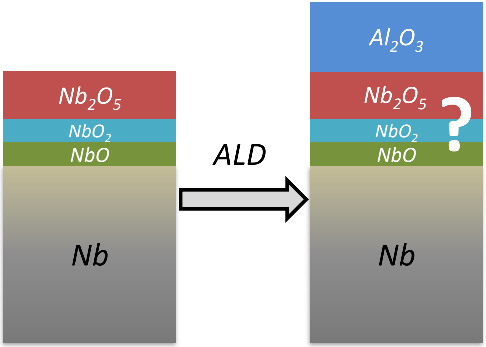

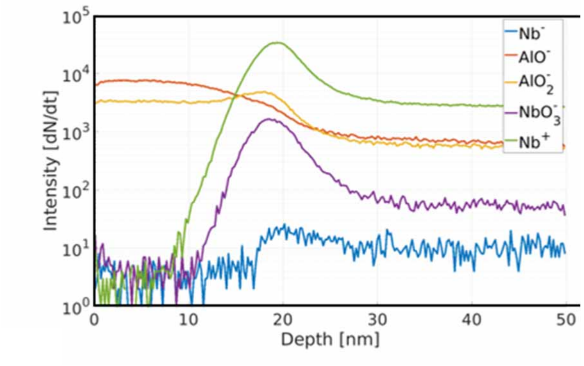

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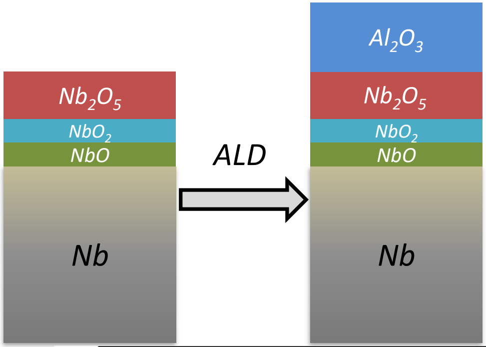

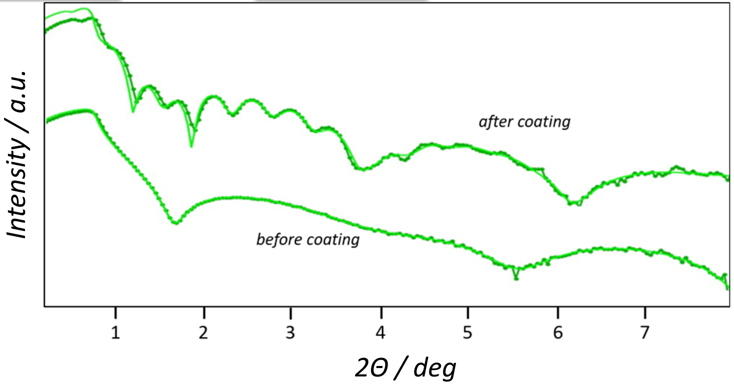

ex-situ	Baseline / Å	After Coating / Å
NbO	9	8
NbO_2	6	10
Nb_2O_5	20	18
Al_2O_3	-	172

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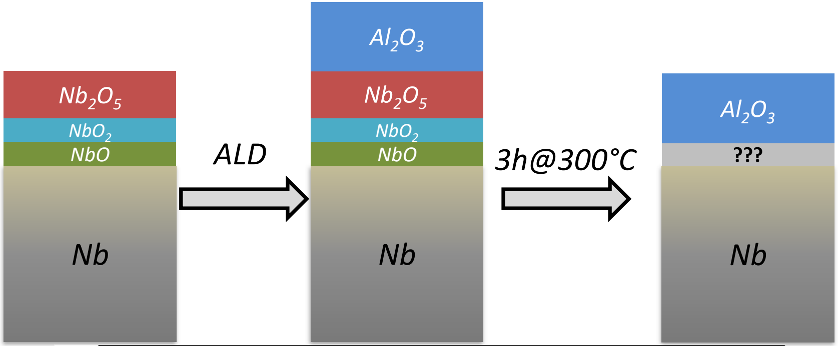

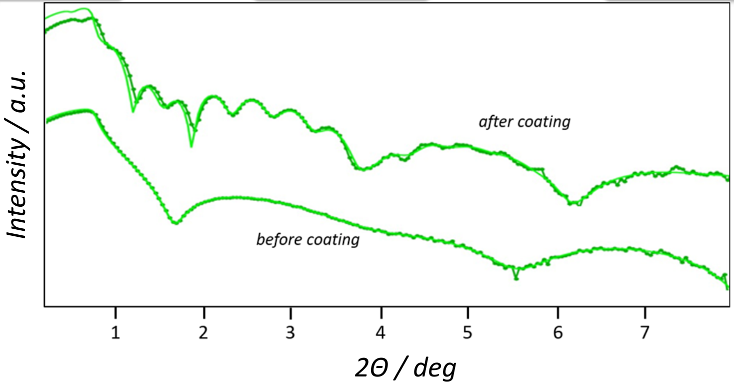

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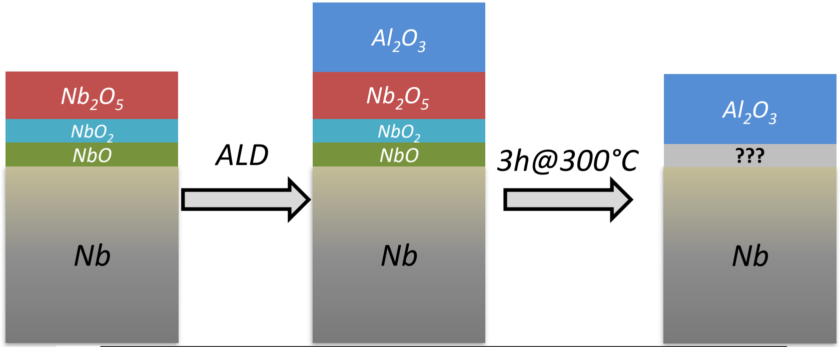
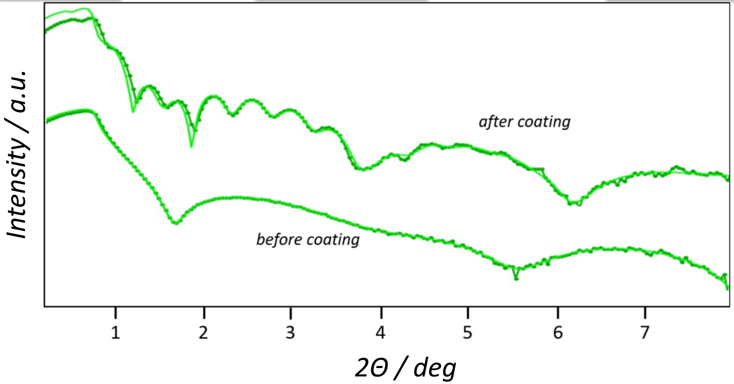
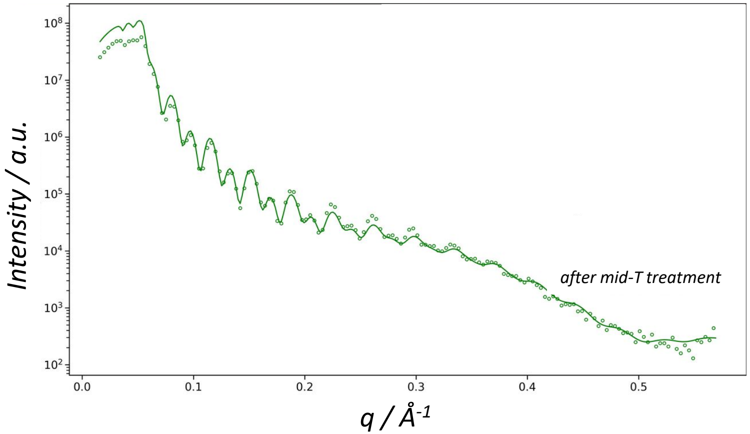
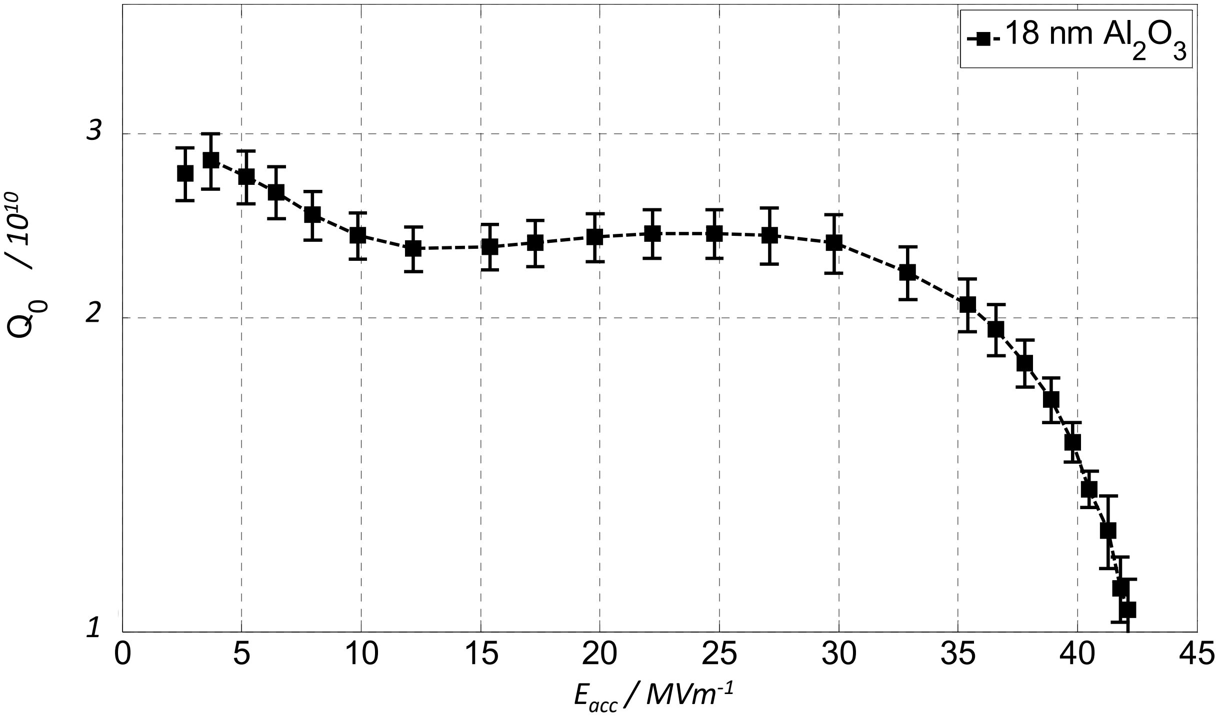






ex-situ	Baseline / Å	After Coating / Å	After mid-T / Å
NbO	*9*	*8*	*12*
NbO_2	*6*	*10*	-
Nb_2O_5	*20*	*18*	-
Al_2O_3	-	*172*	*170*

Mid-T heat treatment of a coated cavity



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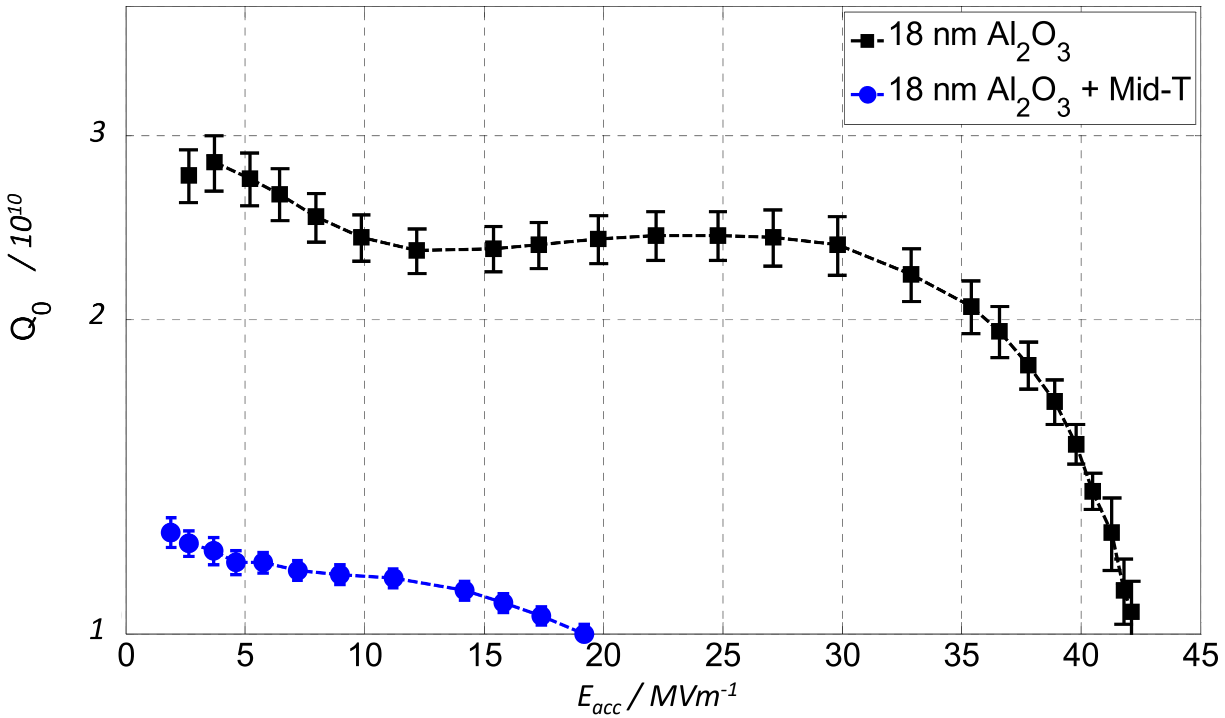

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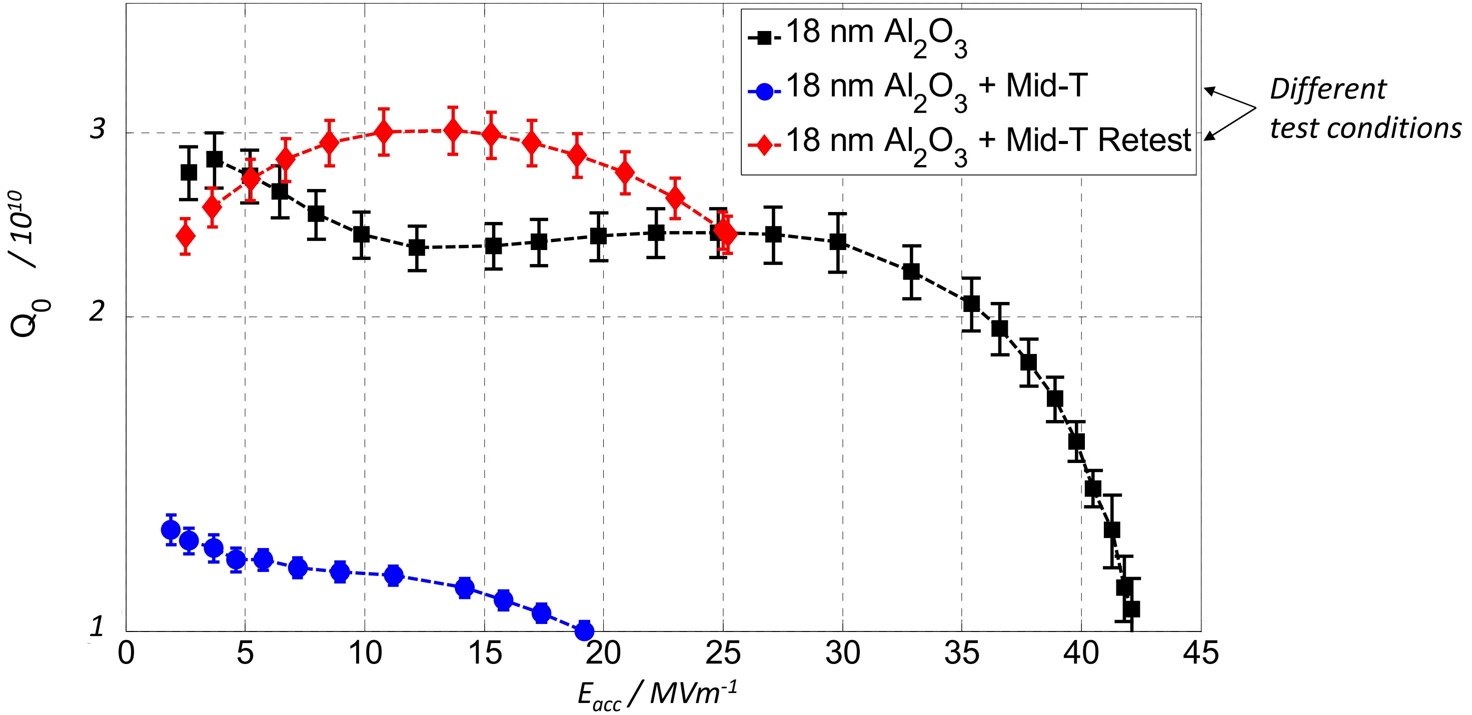

Reduced R_{BCS} beyond regular mid-T cavities

Bate - **MOPMB022**

Ghanbari - **MOPMB021**

- $R_{BCS}(2K) \approx R_S(2K) - \underbrace{R_S(1.5K)}_{\approx R_{res}}$

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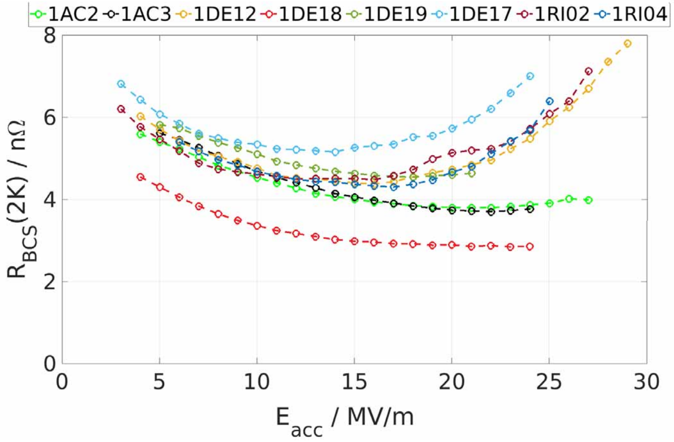
  3nΩ @ 2K
- R_{res} *is higher due to mid-T*

  before: 3nΩ

  after: 6nΩ



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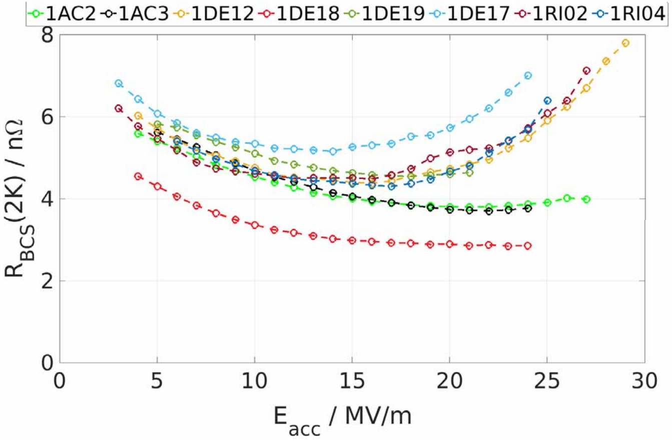
- *R_{res} is higher due to mid-T*
  before: 3nΩ
  after: 6nΩ
- *Why is R_{res} higher?*
  - sensitivity higher for mid-T cavities → increased R_{flux} ?
  - agrees with low Q_0 in first test after mid-T
  - 120°C before mid-T may affect R_{res} negatively



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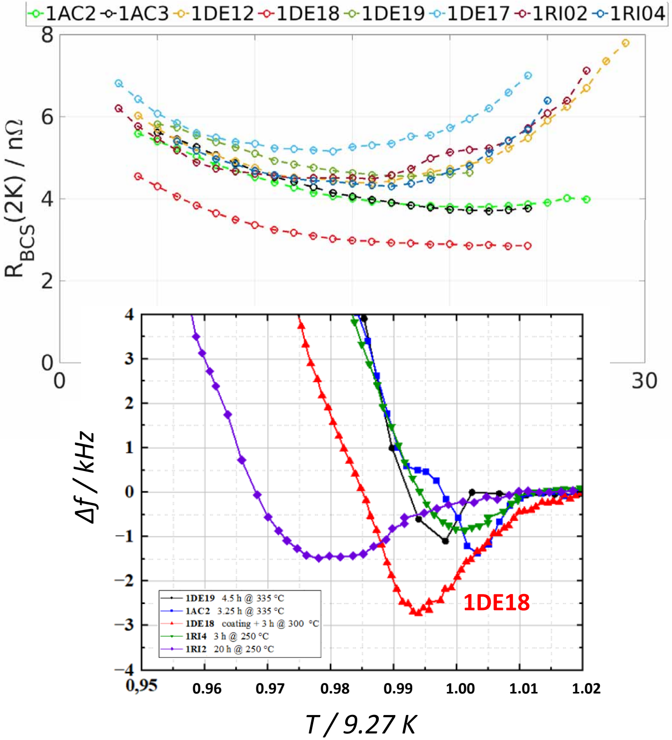
- *f vs. T: dip also differs from „typical“ mid-T*



Summary

- *Nb oxide contains significant amount of oxygen vacancies*
  - causes surface magnetism
  - bound but 'free' electrons (dangling bonds) act as magnetic impurities and TLS

- *Mid-T heat treatment affects cavities in multiple ways*
  - oxide dissociation → interstitial oxygen diffusion
  - oxide reorganization

- *Preventing* Nb_2O_5 *to (re)grow*
  - increases coherence time
  - improves R_{BCS} *to a record value of 3nΩ at 2K & 1.3 GHz*

Thank you

Thanks to

Martin Aeschlimann (TUKL), Christopher Bate (DESY), Robert Blick (UHH), Maik Butterling (HZDR), Jakub Cizek (U Prague), Arti Dangwal-Pandey (DESY), Getnet Deyu (UHH), Alexey Ermakov (DESY), Jürgen Eschke (DESY), Rezvan Ghanbari (UHH), Erik Hirschmann (HZDR), Wolfgang Hillert (UHH), Arno Jeromin (DESY), Thomas Keller (UHH), Nicolay Krupka (DESY), Anton Lorf (UHH), Kay Jensch (DESY), Thomas Keller (DESY), Oskar Liedke (HZDR), Lutz Lilje (DESY), Cornelius Martens (UHH), Giso Marquardt (DESY), Tami Meyer (UHH), Ricardo Monroy-Villa (UHH), Trupen Parik (DESY), Lea Preece (UHH), Detlef Reschke (DESY), Cem Saribal (UHH), Jörn Schaffran (DESY), Marco Schalwat (DESY), Nils Schäfer (TUDA), G.D.L. Semione (U Bremen), Sven Sievers (DESY), Lea Steder (DESY), Martin Stiehl (TUKL), Andreas Stierle (DESY), Antonio Speyer (DESY), Vedran Vonk (DESY), Birte van der Horst (DESY), Andreas Wagner (HZDR), Nick Walker (DESY), Hans Weise (DESY), Artem Zaidman (UHH), Robert Zierold (UHH), Zanon R.I. and many more