Oxide Dissolution and Oxygen Diffusion Scenarios in Niobium and Implications on the Bean–Livingston Barrier in Superconducting Cavities

Work presented is based on our paper in Journal of Applied Physics:

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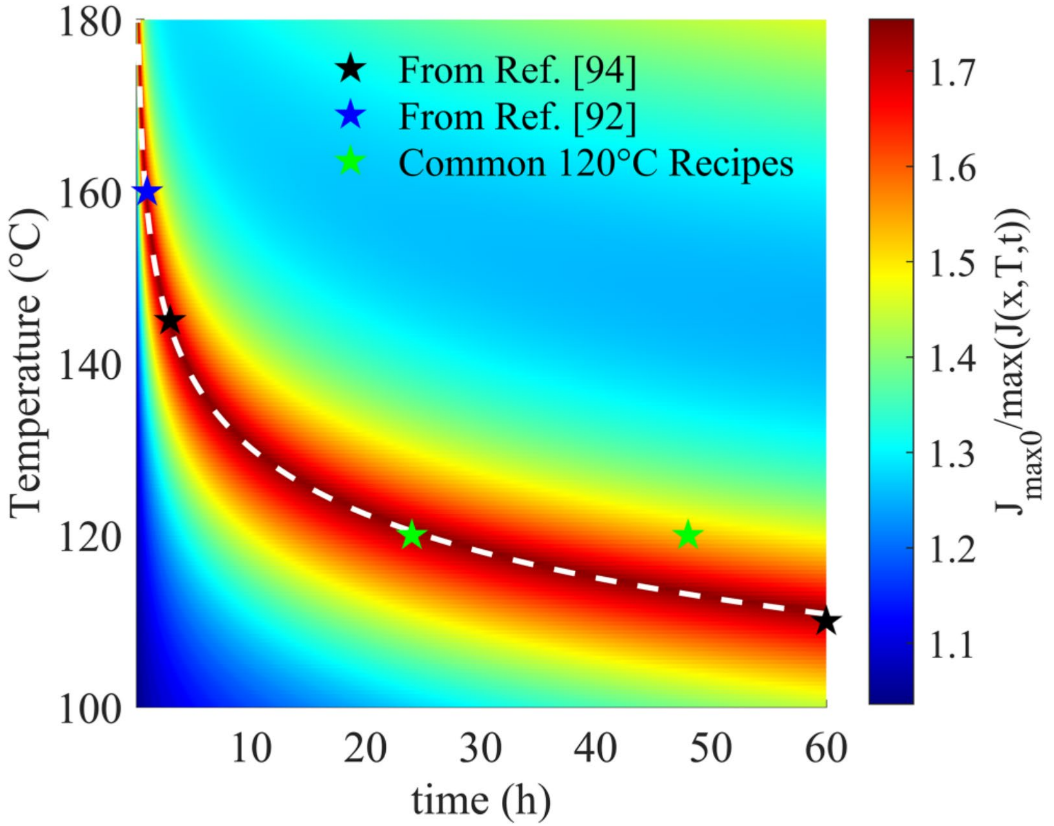
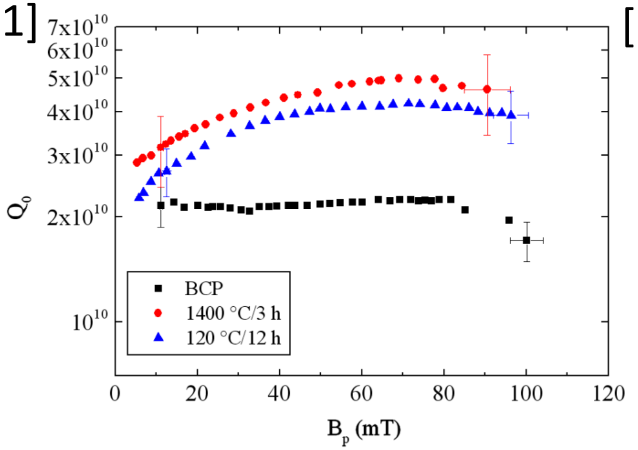


Eric M. Lechner

Introduction – Importance of Impurities

[1]



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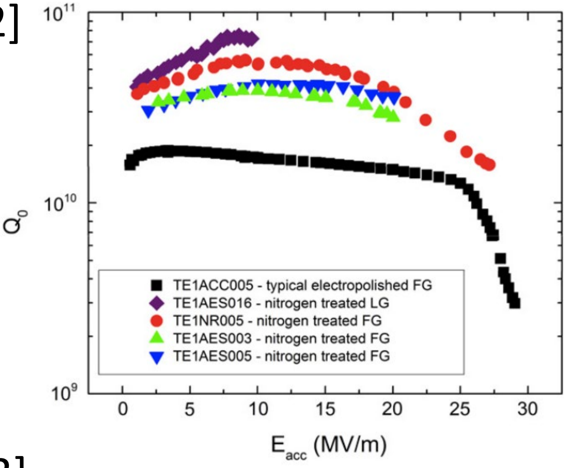

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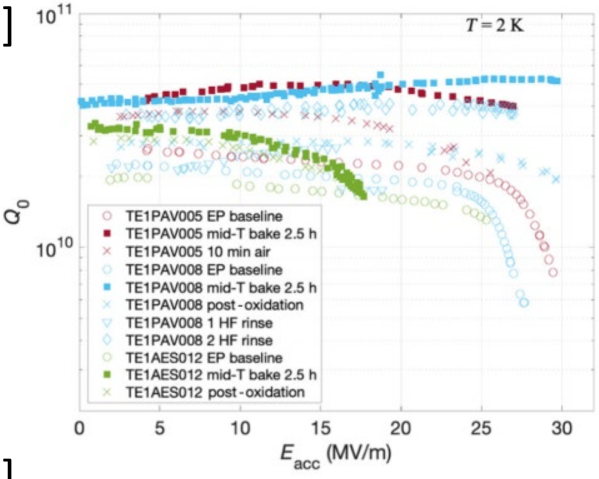
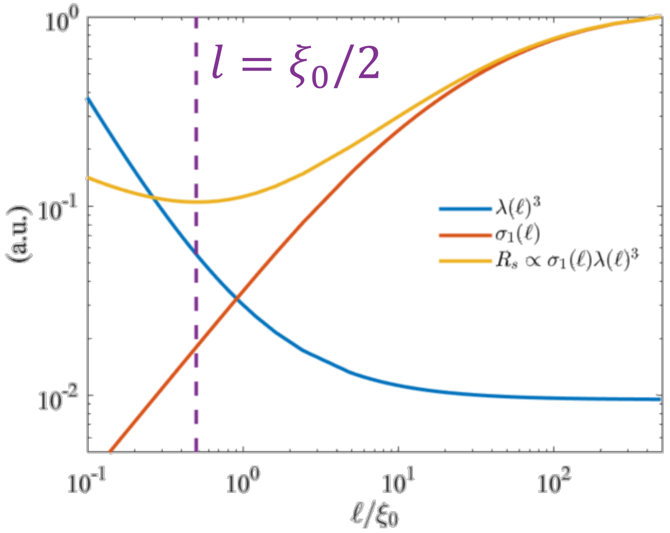
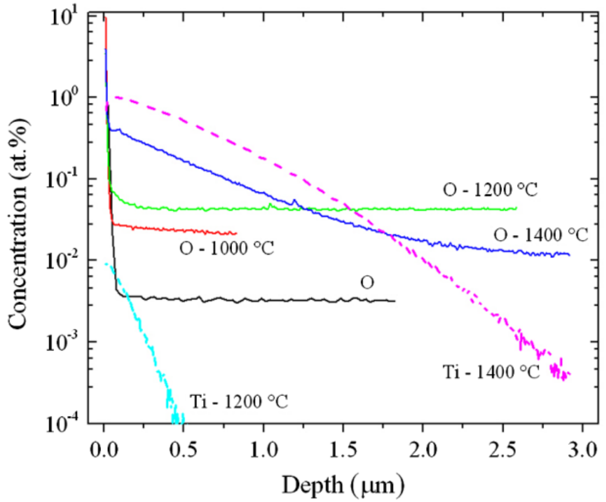


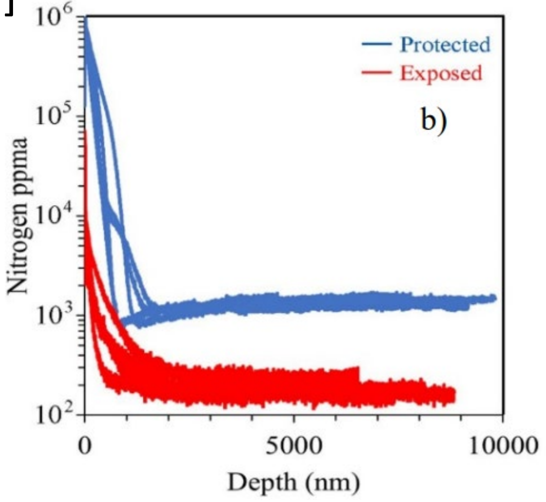
Calculated from [6]





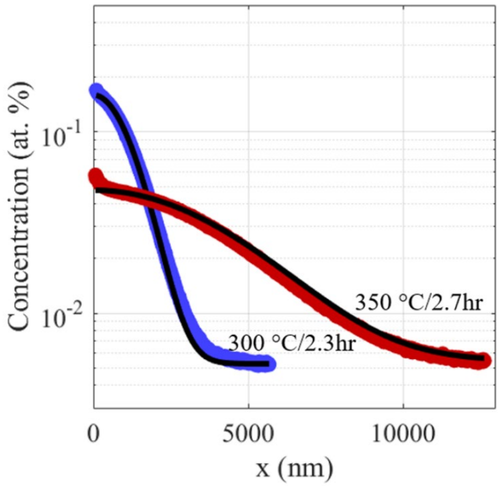
Ti impurities

[3]



N impurities

[5]



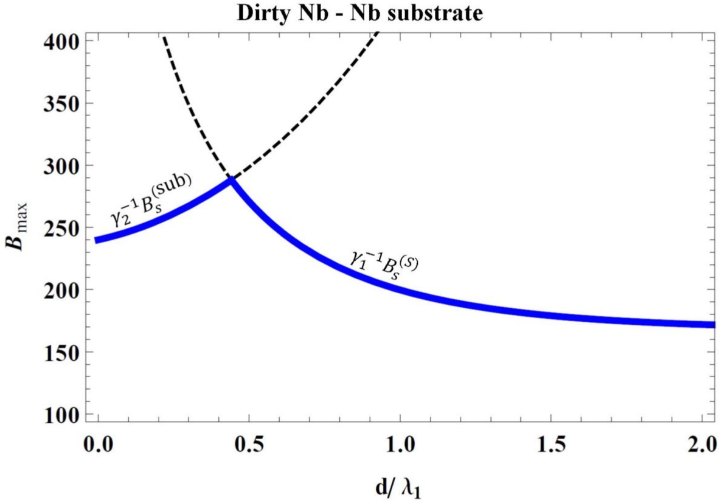
O impurities

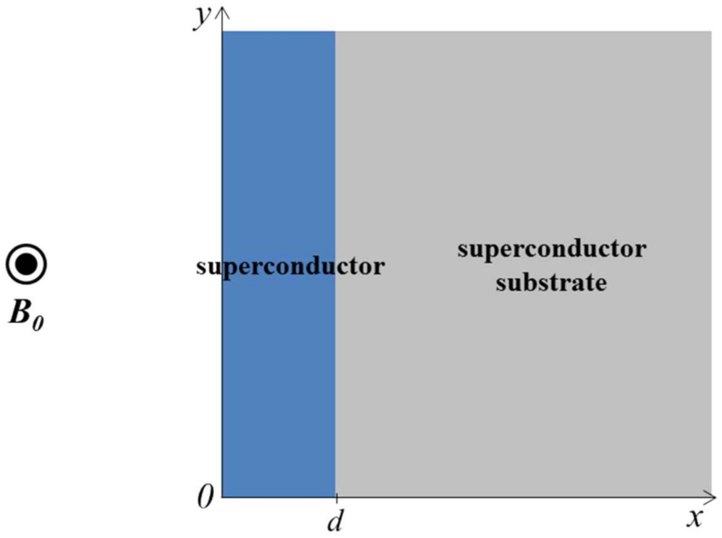
- Impurities are effective for reducing the surface resistance.
- Reduction of R_s arises from a competition of diminishing conductivity and lengthening penetration depth.
- Successfully implemented N-doping in LCLS-II

[1] Dhakal, P., et al. *Physical Review Special Topics-Accelerators and Beams* 16.4 (2013): 042001.
[2] Grassellino, Anna, et al. *Superconductor Science and Technology* 26.10 (2013): 102001.
[3] Reece, Charles, et al. *Challenges to Reliable Production Nitrogen Doping of Nb for SRF Accelerating Cavities*. IPAC2022, 2022.
[4] Posen, S., et al. *Physical Review Applied* 13.1 (2020): 014024.
[5] Lechner, E. M., et al. *Applied Physics Letters* 119.8 (2021).
[6] Kubo, Takayuki. *Physical Review Applied* 17.1 (2022): 014018.

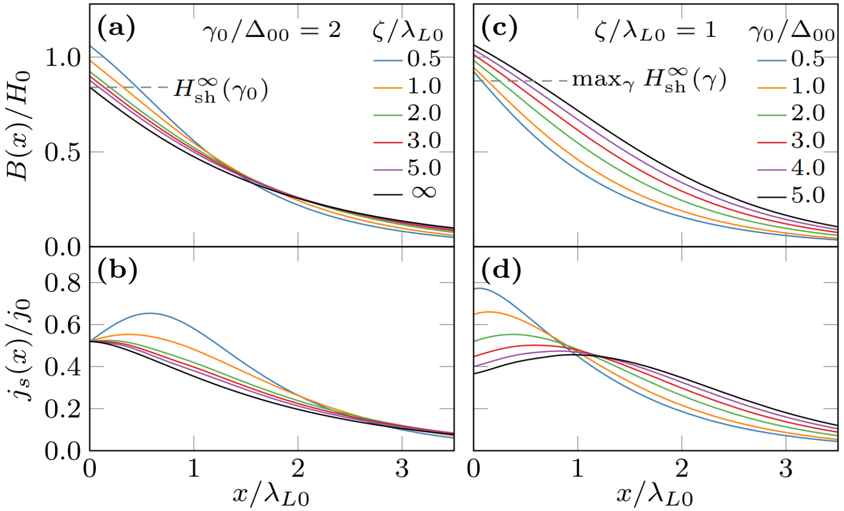
Introduction – Nanostructuring For Boosting E_{acc}

[1] SS bilayer





[2] Thin Impurity Profile



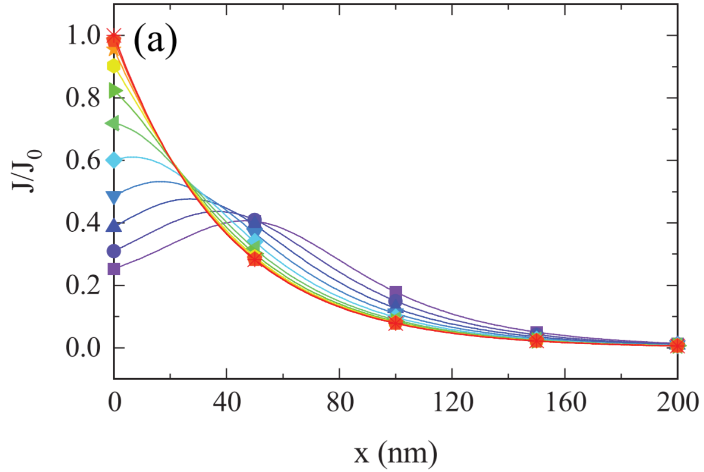
Impurity distribution

$$n_{\mathrm{imp}}(x) = n_0 \exp\left(-x/\zeta\right)$$

Equivalent depth-dependent scattering rate

$$\gamma(x) = \gamma_0 e^{-x/\zeta}$$

[3] Current Redistribution Due to Impurities



$$\lambda^2 B''(x) + 2\lambda\lambda' B'(x) - B(x) = 0$$

$$\lambda(x) = (\lambda_s - \lambda_0)\mathrm{Erfc}\left[\frac{x}{\delta}\right] + \lambda_0$$

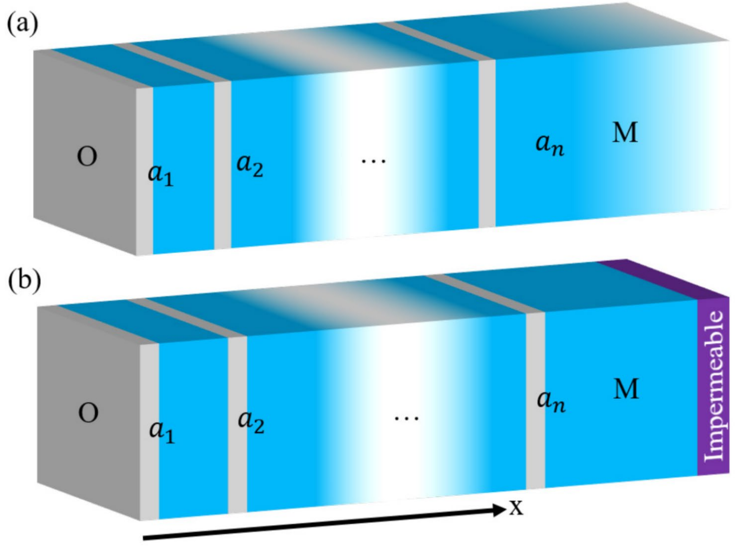
Previously used to shift supercurrent away from the surface (x=0) to protect from possible hydrides, but is essentially a model that can be used instead to examine peak spatial supercurrent. More on this later…

[1] Kubo, T. Superconductor Science and Technology 30.2 (2016): 023001.
[2] Ngampruetikorn, V., and J. A. Sauls. Physical Review Research 1.1 (2019): 012015.
[3] Checchin, M., and A. Grassellino. Applied Physics Letters 117.3 (2020).

Oxide Dissolution & O Diffusion

$$Nb_2O_5 \xrightarrow{k_1} 2NbO_2 + O \xrightarrow{k_2} 2NbO + 3O.$$

$$-\frac{dA}{dt} = k_1 A; \quad -\frac{dB}{dt} = k_2 B - 2k_1 A; \quad -\frac{dC}{dt} = -k_2 B,$$



Explicit Assumption:

1. Diffusion lengths through oxides is larger than oxide thickness. Availability of O to the substrate is not limited by mass transport through the oxide. Otherwise boundary conditions at each oxide need to be considered.

$$\frac{\partial c(x,t)}{\partial t} = D(T)\frac{\partial c(x,t)}{\partial x^2} + \sum_X q_X(x,t)$$

Semi-infinite slab

$$\frac{\partial c}{\partial t} - D\frac{\partial c}{\partial x^2} = \sum_{k=-\infty}^{\infty}\sum_{n=1}^{m}\gamma_n(\delta(x + a_n - 2kd) + \delta(x - a_n - 2kd))$$

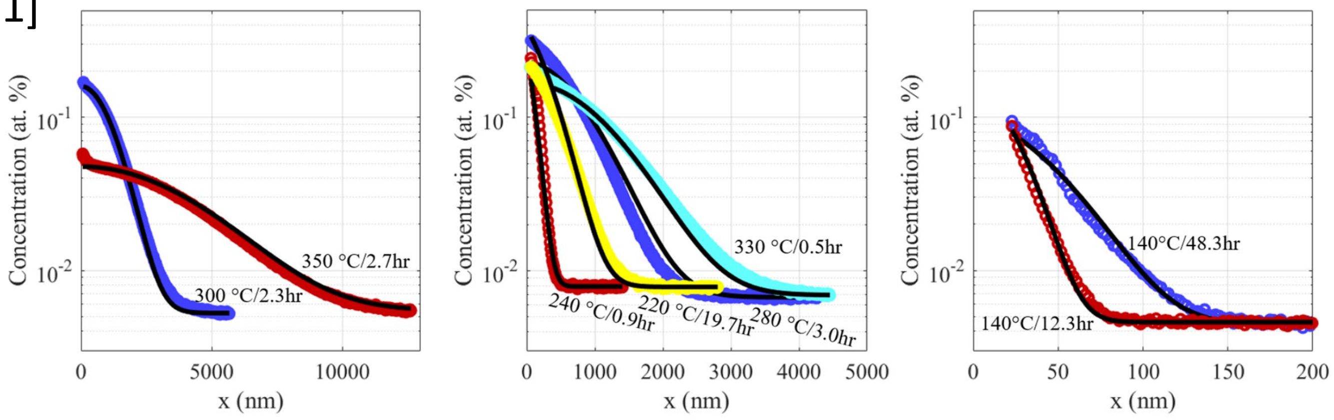
Finite thickness impermeable substrate

$$\frac{\partial c(x,t)}{\partial t} - D(T)\frac{\partial c(x,t)}{\partial x^2} = \sum_{n=1}^{m}\gamma_n(t)(\delta(x + a_n) + \delta(x - a_n))$$

Semi-infinite Single Oxide Layer Dissolution (Nb_2O_5)

$$c(x,t) = \frac{v_0}{\sqrt{\pi D t}}\exp(-x^2/4Dt) + \int_0^t \frac{u_1 k_1 \exp(-k_1 t)}{\sqrt{\pi D(t-s)}}\exp(-x^2/4D(t-s))ds$$

[1]



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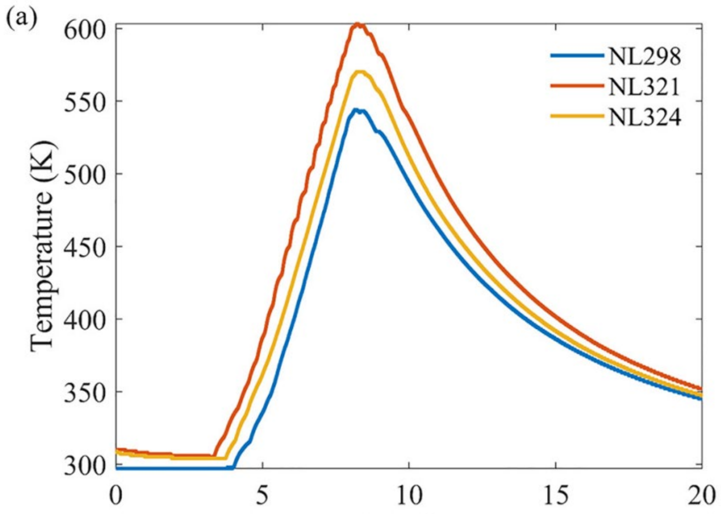
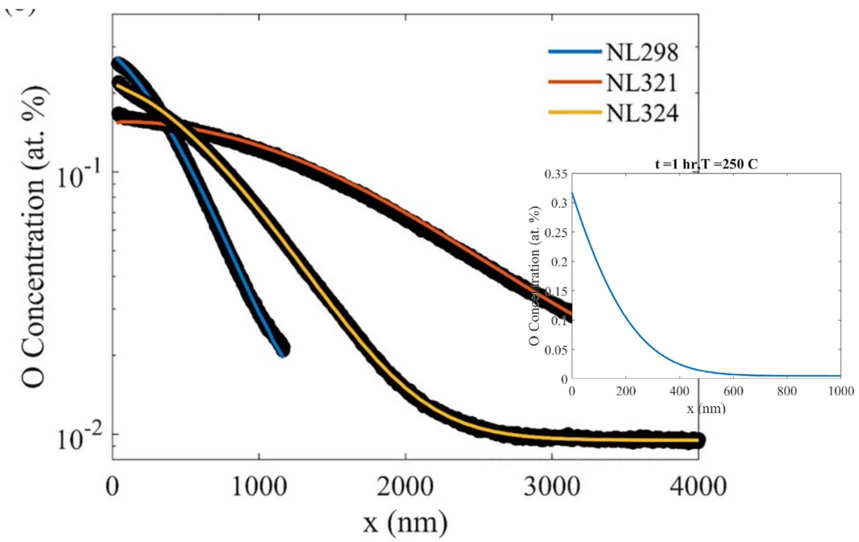
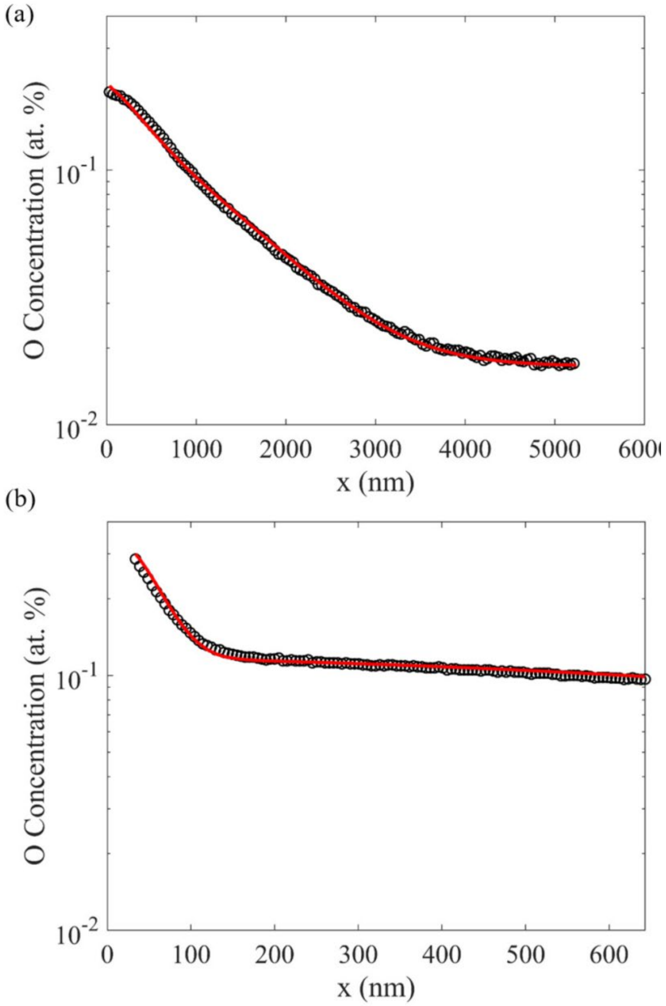
[1] Lechner, E. M., et al. Applied Physics Letters 119.8 (2021).

Short Heat Treatments & Two-step Baking

Short heat treatment (ramp time is considerable)







$$-\frac{dA}{dt} = k_1 A$$

$$-\frac{dA}{dt} \propto q = u_0 k(T(t)) \exp\left(-\int_0^t k(T(s))ds\right)\delta(x)$$

$$\frac{\partial c(x,t)}{\partial t} = D(T(t))\frac{\partial c(x,t)}{\partial x^2} + q(t, T(t))$$

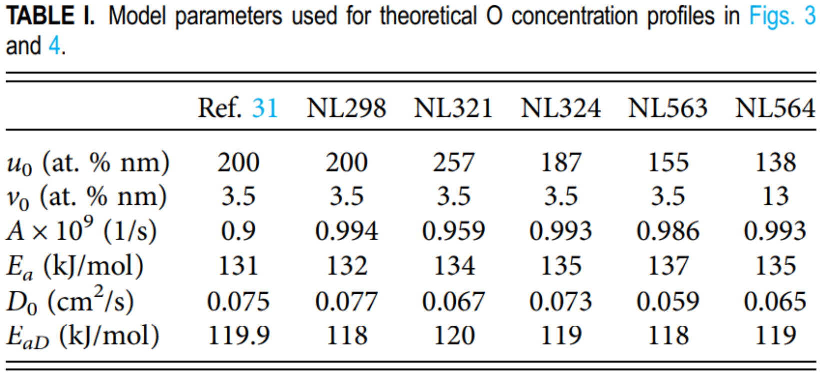


TABLE I. Model parameters used for theoretical O concentration profiles in Figs. 3 and 4.

	Ref. 31	NL298	NL321	NL324	NL563	NL564
u_0 (at. % nm)	200	200	257	187	155	138
v_0 (at. % nm)	3.5	3.5	3.5	3.5	3.5	13
$A \times 10^9$ (1/s)	0.9	0.994	0.959	0.993	0.986	0.993
E_a (kJ/mol)	131	132	134	135	137	135
D_0 (cm^2/s)	0.075	0.077	0.067	0.073	0.059	0.065
E_{aD} (kJ/mol)	119.9	118	120	119	118	119

What's Been Done Previously?

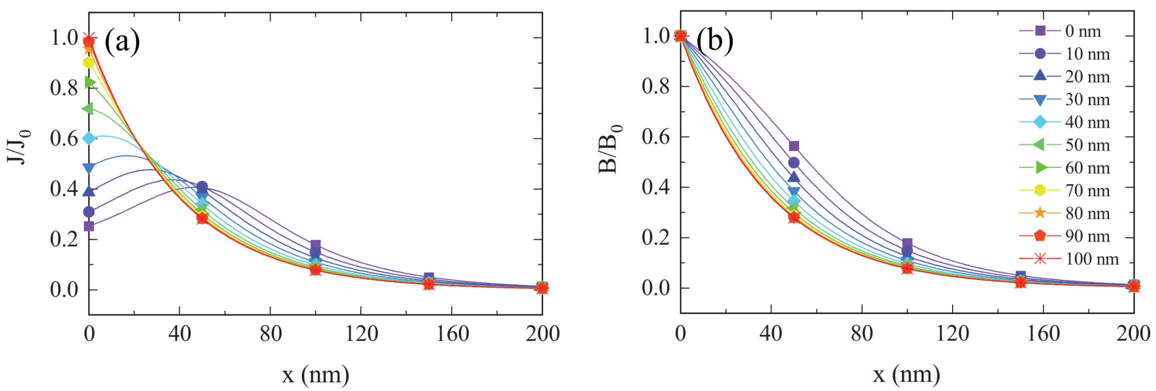


FIG. 2. Simulation of current redistribution for $\delta = 50$ nm, $\lambda_s = 100$ nm, and peak magnetic field for different values of material removal.

Modified London Equation

$$\lambda^2 B''(x) + 2\lambda\lambda' B'(x) - B(x) = 0$$

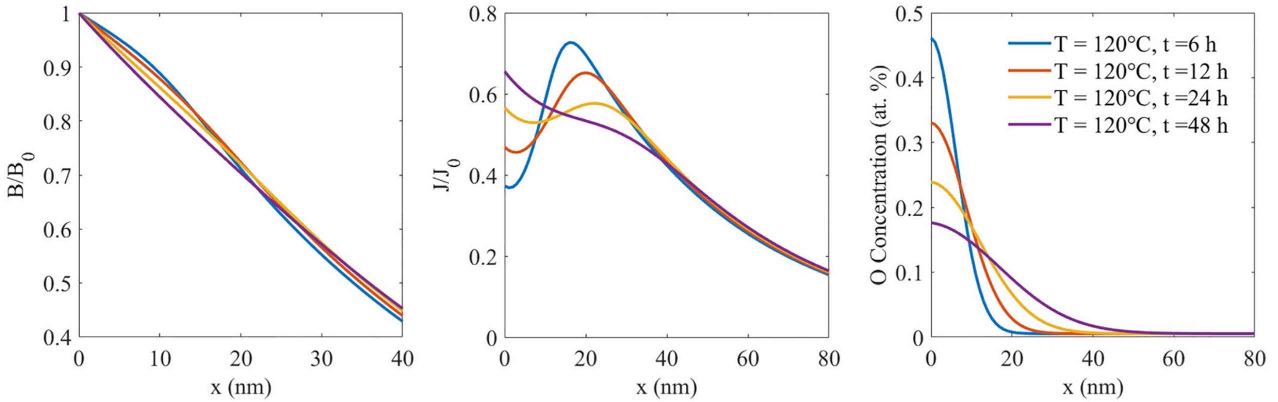
$$\lambda(x) = (\lambda_s - \lambda_0)\mathrm{Erfc}\left[\frac{x}{\delta}\right] + \lambda_0$$

Breakdown condition

Hydride breakdown at surface

$$B'(0) = \mu_0 J_H = -B_{EP}/\lambda_0,$$

Both models are critical field models



Modified London Equation

$$\lambda^2 B''(x) + 2\lambda\lambda' B'(x) - B(x) = 0$$

$$l(x) = \frac{\sigma}{\Delta\rho_O} \quad \lambda(x) = \lambda_0\sqrt{1 + \xi_0/l(x)}$$

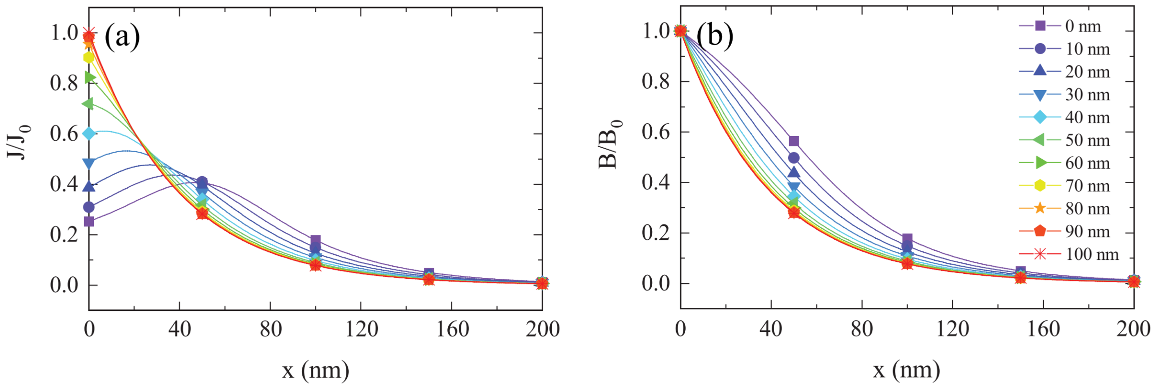
$$c(x,t) = \frac{v_0}{\sqrt{\pi D t}}\exp(-x^2/4Dt) + \int_0^t \frac{u_1 k_1 \exp(-k_1 t)}{\sqrt{\pi D(t-s)}}\exp(-x^2/4D(t-s))ds$$

Breakdown condition

Vortex Nucleation

$$\max(J(x)) = J_d$$

What’s Been Done Previously?



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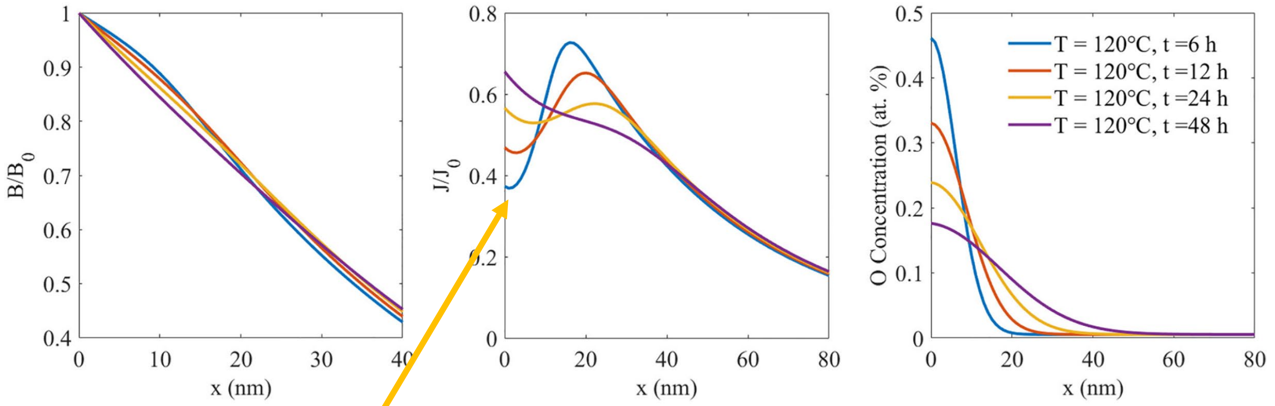

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Breakdown condition

Vortex Nucleation

$$\max(J(x)) = J_d$$

Consideration:

In the present O diffusion model, strongest suppression of the supercurrent density at the surface occurs for short treatments. This means very short LTB times should produce the best result in the hydride breakdown model, in contradiction to LTB measurements.

Some Experiments on Low Temperature Baked Nb

[1] Reduction of electron mean free path with baking temperature

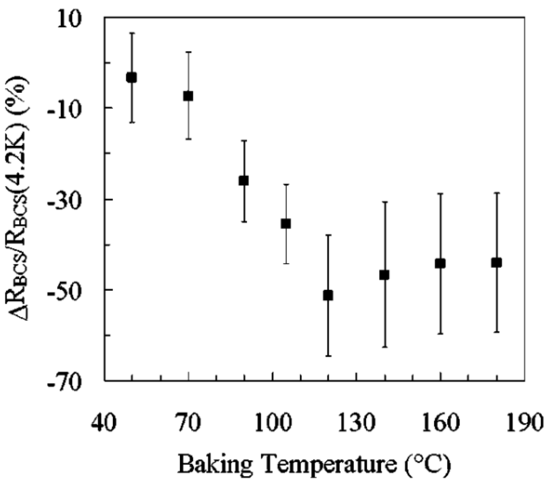


FIG. 8. Variation of BCS surface resistance at 4.2 K as a function of baking temperature.

[2] LTB Effect is localized to ~50 nm depth

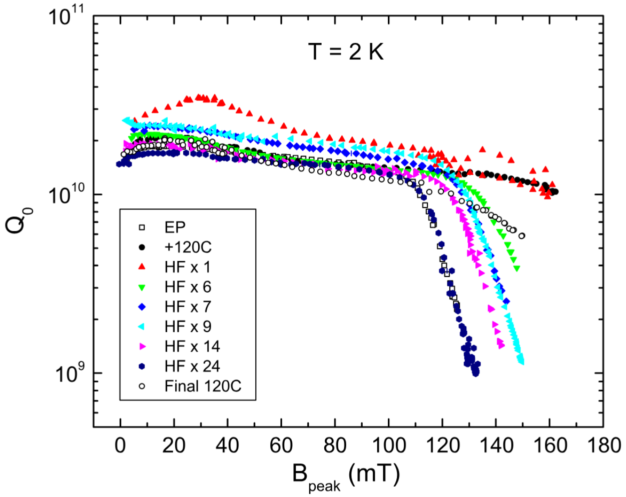
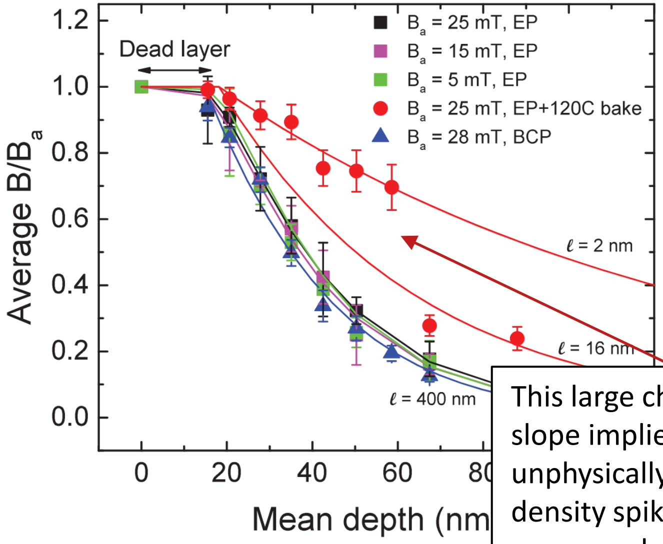


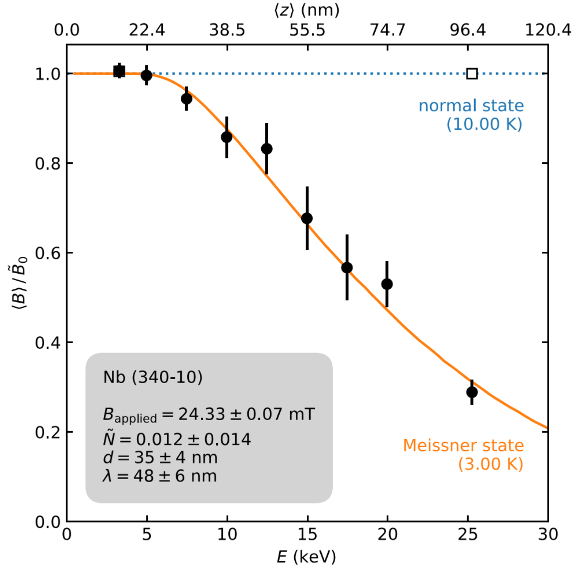
FIG. 3. Cavity rf test results after multiple HF rinse cycles for the electropolished cavity TE1ACC005. No field emission was present except for the final 120°C test.

[3]



This large change in slope implies an unphysically high current density spike within the superconductor.

[4] No obvious discontinuities in Meissner screening profile



[1] Ciovati, G. *Journal of applied physics* 96.3 (2004): 1591-1600.
[2] Romanenko, A., et al. *Physical Review Special Topics-accelerators and beams* 16.1 (2013): 012001.
[3] Romanenko, A, et al. *Applied Physics Letters* 104.7 (2014).
[4] McFadden, RML, et al. *Appl. Phys. Lett.* 19 February 2024; 124 (8): 086101.

Do Thin Impurity Profiles Play a Role In Low Temperature Baked Nb?

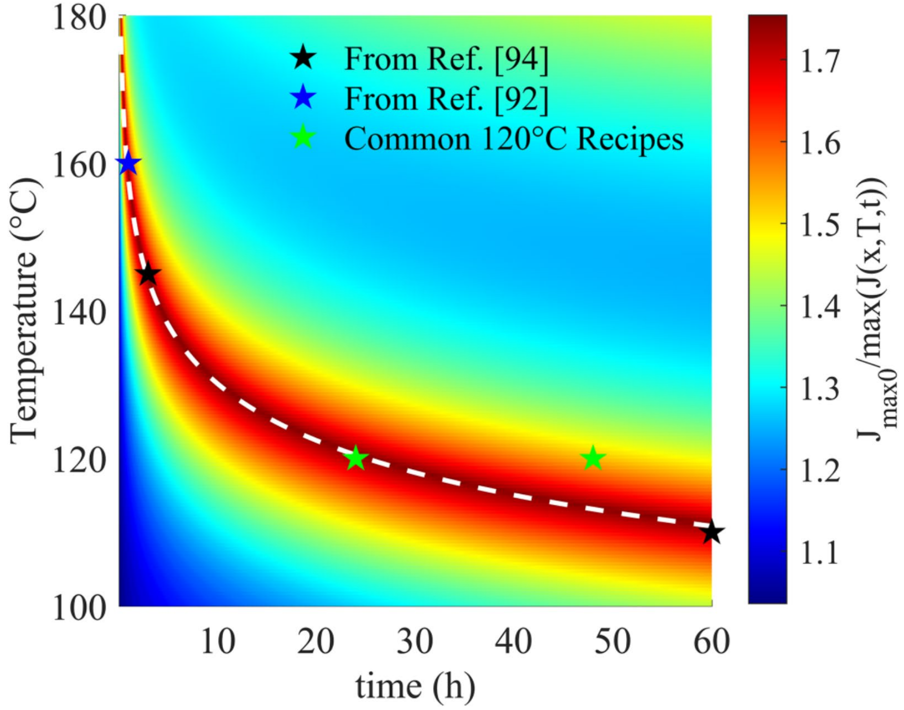
Major O contributor in LTB is the interstitial O at the oxide/metal interface

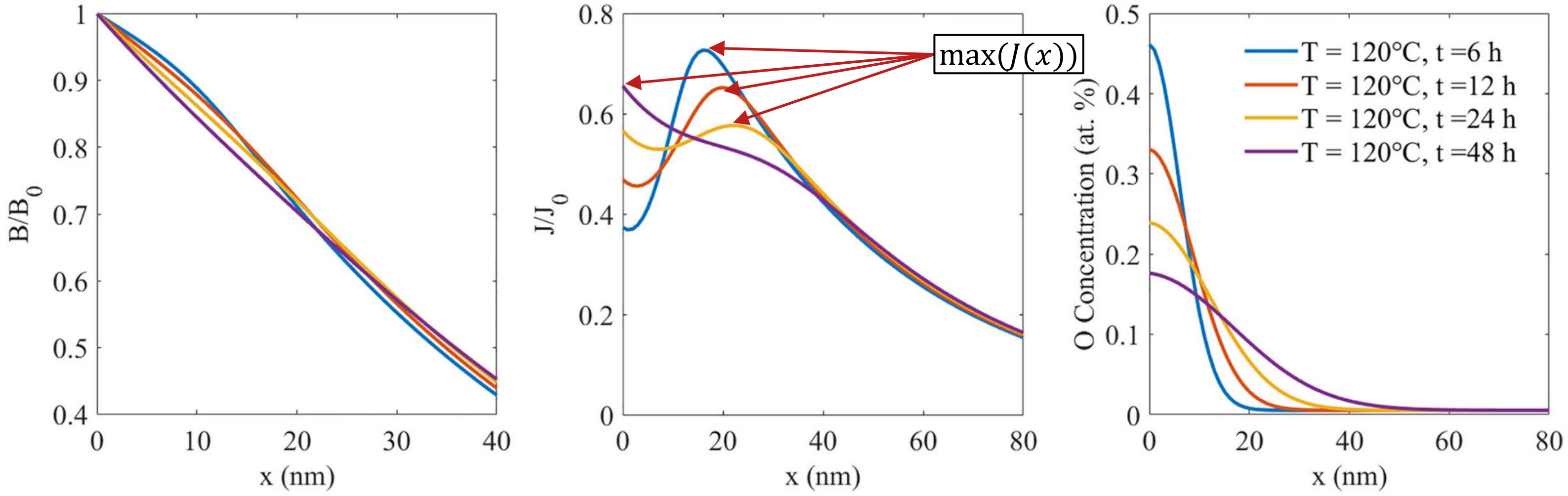
$$\lambda(x)^2 B'' + 2\lambda(x)\lambda'(x)B' = B$$

$$\lambda(x) = \lambda_0\sqrt{1+\xi_0/l(x)} \qquad l(x) = \frac{\sigma}{\Delta\rho_O}$$

$$\sigma = 0.37\times10^{-15}\Omega\,\mathrm{m}^2$$
$$\Delta\rho_O(x) = ac(x)$$
$$a = 4.5\times10^{-8}\Omega\,\mathrm{m}$$

$$\lambda_0 = 39\ \mathrm{nm}$$
$$\xi_0 = 38\ \mathrm{nm}$$



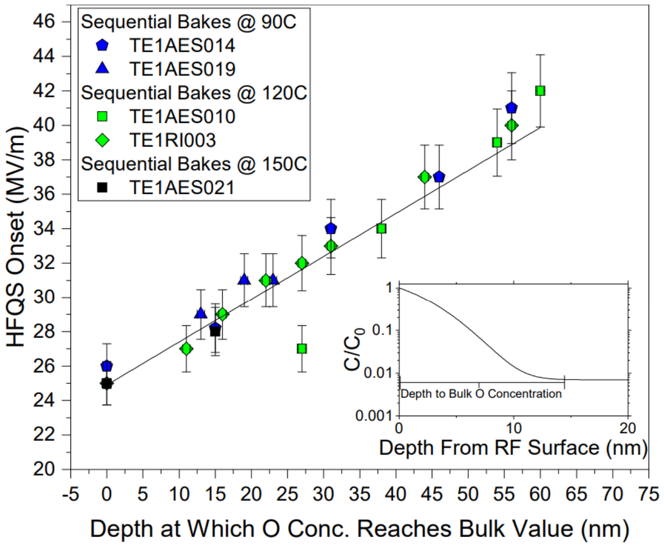


Reasonably describes the locations of HFQS ameliorating heat treatment times and temperatures.

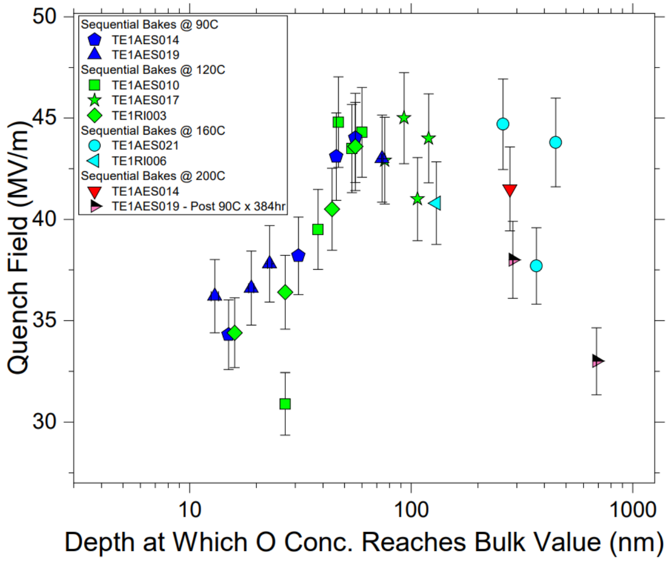
$$E_q = E_{q0}J_{\max 0}/\max\left(J(x,\,T,\,t)\right).$$

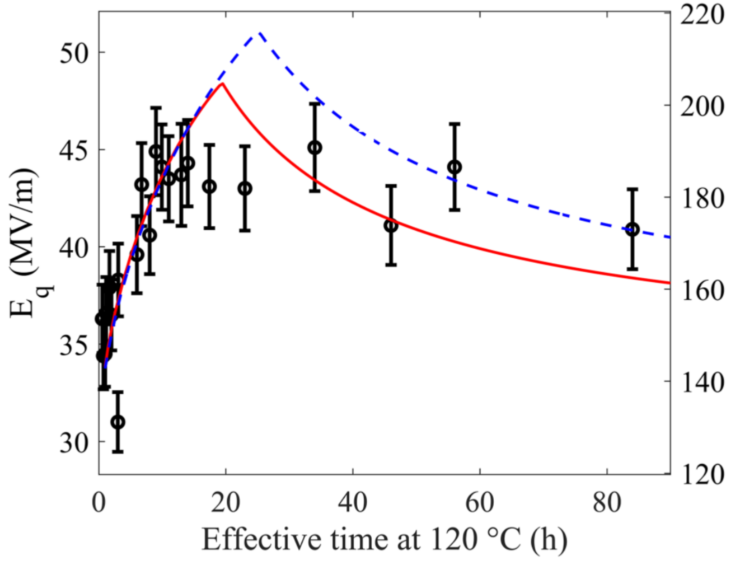
Quench Field Measurements

[1]



[1]





$$E_q = E_{q0} J_{\max 0} / \max\left(J(x, T, t)\right).$$

Best fit to Bafia et al.

$E_{q0} = 29.2$ MV/m

$\nu_0 = 2.6 \pm 0.3$ at. % nm

Estimate from Lechner et al.

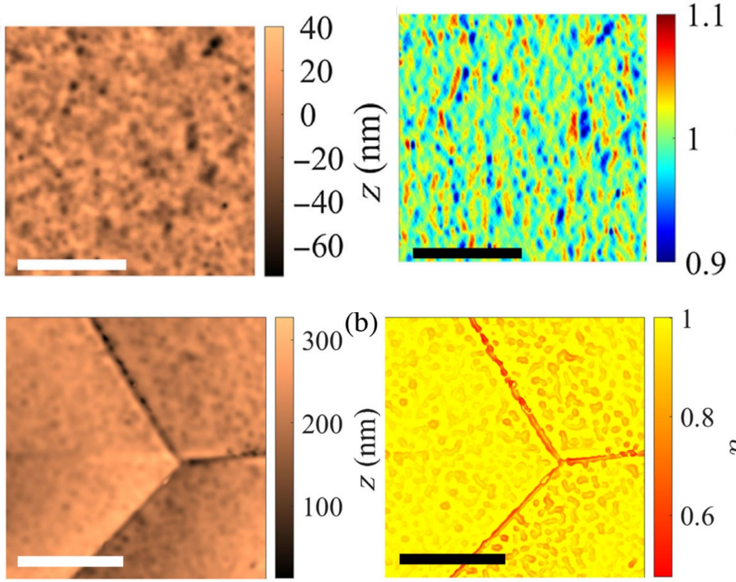
$E_{q0} = 29.2$ MV/m

$\nu_0 = 3.5$ at. % nm

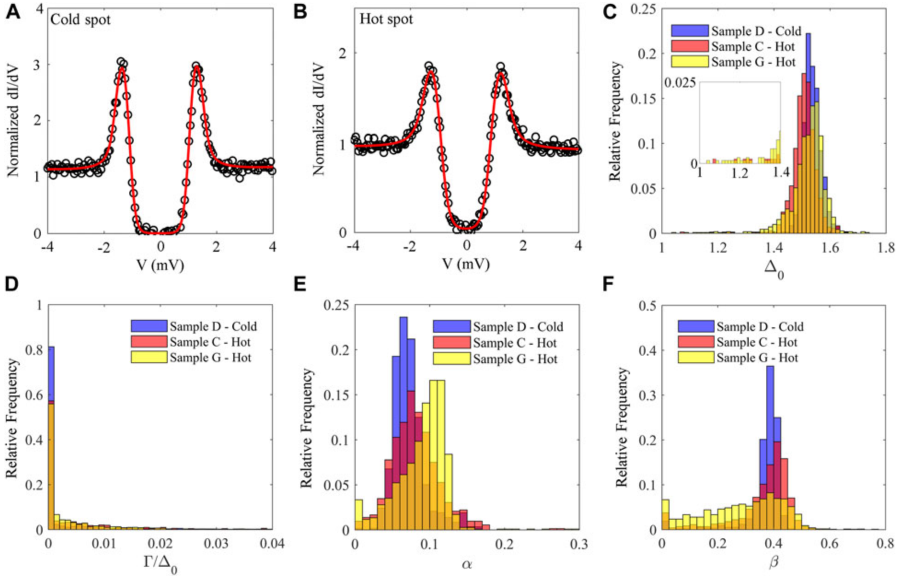
[1] Bafia, D., et al. SRF’21, 2021.

Vortex Nucleation Scenarios

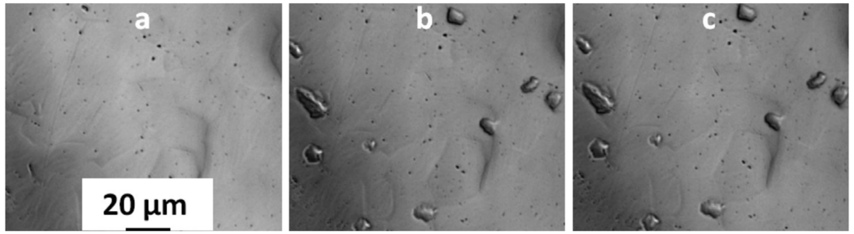
[1] Topographically?



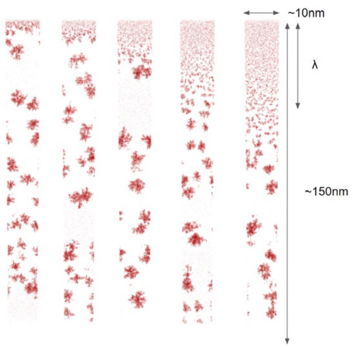
[2] Weakened Superconductivity?

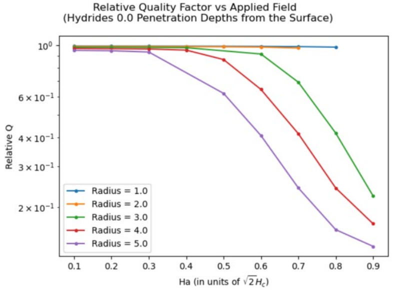


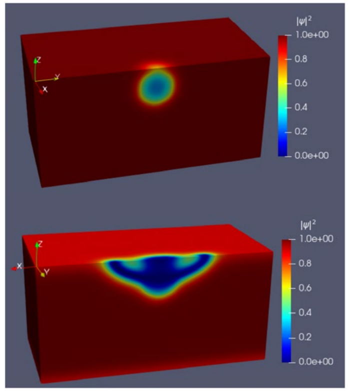
[3] Nano hydrides?



[4]







[1] Lechner, Eric M., et al. *Physical Review Accelerators and Beams* 26.10 (2023): 103101.
[2] Lechner, Eric M., et al. *Frontiers in Electronic Materials* 3 (2023): 1235918.
[3] Barkov, F., et al. *Journal of Applied Physics* 114.16 (2013).
[4] Sitaraman, N. S., et al. *SRF'23 (*2023).

Conclusions

- Further developed a model to describe O migration in multi-component, multilayer decomposition.
- Time dependent temperature single layer dissolution and multistep process models developed and tested against SIMS measurements.
- A model for peak supercurrent suppression based on the modified London equation and O diffusion is proposed. It is found to reasonably describe the T-t distribution of HFQS ameliorating heat treatments. It is in reasonable agreement with the measurements of Bafia et al.

Acknowledgments

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