Defect profile engineering in Nb for SRF accelerator applications: Simulating the dissolution and diffusion of Nb's surface oxide layer

by

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ABSTRACT

Superconducting radio-frequency cavities made from Nb are widely used in particle accelerators due to their ability to sustain strong electromagnetic fields with low energy loss. Their performance is strongly influenced by surface superconducting properties, which can be controlled through heat treatments that introduce interstitial oxygen.

This project models how oxygen diffuses into Nb during baking and how this affects Nb's superconducting behavior. Using the Crank–Nicolson numerical method, we solved a reaction–diffusion equation to simulate oxygen concentration profiles and compute related superconducting quantities such as the magnetic penetration depth and supercurrent density.

By simulating thousands of recipes, we analyzed how different baking conditions influence performance. We evaluated the recipes by three metrics: peak and surface supercurrent, and the depth of the supercurrent peak.

The results show that quantifying an optimized recipe must take into account multiple metrics. We also found a limit for baking conditions beyond which the peak supercurrent can no longer be pushed into the bulk Nb. This work provides the basis of a framework for understanding and improving heat treatments for Nb cavities as they relate to SRF particle accelerators.

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Chapter 1

Introduction

The main focus of this honours project is the optimization of superconducting radio-frequency (SRF) cavities, which are crucial components in particle accelerator technology. While experimental work has improved cavity performance over the past decades [21], many methods rely on empirical recipes - a certain time and temperature combination - discovered through trial and error. By taking a theoretical simulation approach this project aims to provide a way to enhance the cavity performance in a more systematic and scalable way.

Improving SRF cavities has important implications for both fundamental research and applied science. These cavities typically made out of niobium (Nb) are responsible for transferring electromagnetic energy into kinetic energy, enabling the acceleration of higher energy particles. Optimized cavities increase accelerating gradients, reducing operational costs, and improving accelerator footprints.

A numerical simulation approach is taken, using a finite difference method (fdm) to explore heat treatment conditions for optimizing Nb cavities. Specifically, this work develops a software package that simulates oxygen dissolution and diffusion dynamics under a wide range of treatment parameters, while computing useful and relevant quantities. This provides the ability for future researchers to test hypotheses and refine recipes without the need to physically bake Nb samples which is time consuming and costly.

The main ideas of this project include the application of the Crank–Nicolson (CN) method to solve the oxygen dissolution and diffusion equations in Nb [16], as part of a codebase facilitating simulations over a wide range of treatment conditions, giving the ability to efficiently explore the problem parameter space. These simulations make it possible to track how oxygen concentration profiles evolve in the near-surface

region (∼5 nm) during vacuum heat treatments and how these profiles impact superconducting performance [19].

Initial results have provided information on the relationship between treatment conditions and cavity performance. In particular, the simulations enable the setup for quantifying the performance for a given recipe, and show a clear limit where heat treatments provide optimal doping profiles and increased cavity performance.

1.1 Agenda

- **Chapter 1** contains an introduction to the project's scope and outlines the core ideas, goals, and claims of the work.
- **Chapter 2** introduces the background and theory of SRF cavities. It emphasizes the importance of niobium SRF cavities for particle accelerators and discusses how heat treatments introduce interstitial oxygen to improve superconducting performance. The surface reduction reactions governing this process are described, and Lechner's PDE model, which captures this process, is presented to frame the optimization problem in terms of solving a PDE.
- **Chapter 3** describes how the reaction–diffusion equation from Chapter 2 is solved using the Crank–Nicolson method, a stable and accurate numerical method. This allows us to simulate how oxygen diffuses into Nb during baking and compute useful superconducting properties, which are further described in this section.
- **Chapter 4** presents the results and analysis from the numerical simulations. It first looks at a single heat treatment recipe (120°C for 6 hours) and shows how the resulting oxygen profile changes Nb's superconducting properties, most importantly, the supercurrent distribution. Then thousands of recipes across time and temperature values are analyzed, showing how different recipes affect peak supercurrent, surface supercurrent, and the depth at which the supercurrent peak occurs. By considering these metrics, we show what constitutes an optimized recipe and how there is a clear limit to the depth the peak can be pushed into the bulk of Nb.
- **Chapter 5** Goes over the discussion and presents the conclusions from the work.

- **Chapter 6** summarizes the projects contributions and outlines future directions.

Chapter 2

Optimizing Nb Cavities

Superconducting radio-frequency accelerators rely on the ability to generate and sustain strong electromagnetic fields with minimal energy loss. A key component enabling this capability is the superconducting cavity — a resonant chamber typically made from Nb.

2.1 SRF Accelerators and Niobium Cavities

In an SRF accelerator, radio-frequency (RF) fields oscillate within a cavity and particles are sent into the cavity timed in such a way that they align with the phase of the oscillating RF field and experience an energy gain as they pass through. To minimize energy losses, these cavities are constructed from superconducting materials, such as Nb, due to its high superconducting critical temperature ($T_c \approx 9.7 \pm 0.6$ K)[26].

When cooled below its critical temperature, Nb transitions into a superconducting state and expels magnetic fields from its bulk (the Meissner effect). However, RF fields can still penetrate the surface, resulting in flux vortices and energy to be lost from the cavity. This means the cavity performance is critically sensitive to the material surface composition and needs to be engineered accordingly.

2.2 Heat Treatments: Baking of Nb Cavities

A common method to engineer Nb, thereby enhancing surface performance, is heat treatments in vacuum ovens. This is done by first exposing the Nb sample to air and doping the near surface region ($\sim$5 nm) then baking the sample for a given

"recipe" (time and temperature). This process introduces oxygen intersitials into the niobiom, resulting in an inhomegeneous oxygen concentration profile, affecting the superconducting properties of Nb. By fine tuning the oxygen concentration profile we are able to control the screening profile and supercurrent density, allowing the Nb to store higher amounts of energy without loss.

Low-temperature baking is a common regime typically conducted at 120°C for 24–48 hours. It has been shown to reliably reduce the Q-drop at high accelerating gradients [6]. This improvement, initially discovered empirically, is most likely due to a set of chemical reactions involving oxygen species in the near the surface region of the cavity.

The reaction reduction process can be described as follows: native Nb pentoxide (Nb_2O_5) exists as a thin surface oxide layer due to air exposure. During baking, this oxide undergoes a reduction reaction, releasing oxygen into the Nb sample. The main chemical reactions can be represented as:

$$\begin{aligned} Nb_2O_5 &\xrightarrow{k_1} 2NbO_2 + O, \\ NbO_2 &\xrightarrow{k_2} NbO + O, \\ NbO &\xrightarrow{k_3} Nb + O, \end{aligned} \tag{2.1}$$

where k_i is the reaction rate constant.

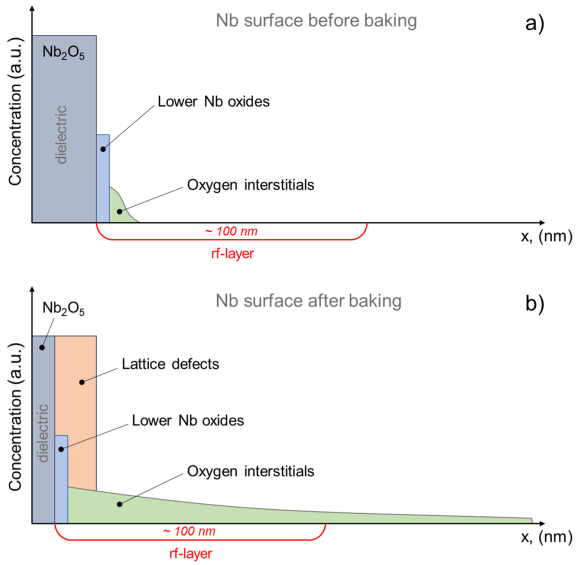

Figure 2.1: Schematic of Surface Layer Oxygen Diffusion Process [25]

Through this diffusion process interstitial oxygen atoms are introduced into the

near surface region (∼150 nm) as seen above, altering the material makeup and modifying the superconducting properties of the Nb in such a way that the cavity performance is increased.

2.3 Modeling the Oxygen Diffusion Process

To better understand and optimize this process, Lechner et al. [16] proposed a reaction–diffusion model that describes the evolution of the oxygen concentration profile during baking. The partial differential equation (PDE) describes Fick's second law of diffusion with a reaction source term:

$$\frac{\partial c(x,t)}{\partial t} = D(T(t))\frac{\partial^2 c(x,t)}{\partial x^2} + q(t,T(t)) \tag{2.2}$$

where $C(x,t)$ is the oxygen concentration as a function of depth x and time t, $D(T)$ is the diffusion coefficient (temperature dependent), and $q(t,T(t))$ is a reaction term describing the rate of oxygen release from the oxide layer. It should be noted that a time dependent temperature was not considered in the simulations and analysis.

This PDE captures the reaction diffusion process, providing a framework to simulate different baking parameters and investigate the resulting oxygen concentration profile. The problem then boils down to how can we efficiently and accurately solve this PDE for a wide array of time and temperature inputs to explore the parameter space of heat treatments as they relate to optimizing Nb cavity performance?

Chapter 3

Solving the Dissolution Diffusion Equation

3.1 Numerical Approach: The Crank–Nicolson Method

To solve the reaction–diffusion PDE introduced in the previous section, we employ the Crank–Nicolson (CN) method, an implicit finite difference method originally developed to solve the heat equation [7].

The CN method discretizes time and space, representing the oxygen concentration $c(x,t)$ on a 2D grid of N_x points in space (with step size Δx) and N_t points in time (with step size Δt). The oxygen concentration is then approximated at each grid point removing the need to solve the PDE analytically.

The PDE

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + q(x,t) \tag{3.1}$$

is discretized using central differences in space and trapezoidal integration in time, giving second-order convergence:

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{D}{2(\Delta x)^2}\left[C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1} + C_{i+1}^n - 2C_i^n + C_{i-1}^n\right] + q_i^n. \tag{3.2}$$

Rearranging terms, the discretized system at each time step takes the form:

$$\mathbf{A}\mathbf{C}^{n+1} = \mathbf{B}\mathbf{C}^n + \Delta t\,\mathbf{Q}^n, \tag{3.3}$$

where $\mathbf{A}$ and $\mathbf{B}$ are tridiagonal matrices containing coefficients derived from the CN

method which define the spread of oxygen from one spatial grid to the next and $\mathbf{Q}^n$ is the reaction source vector at time step n.

The solution is generated iteratively, solving at each time step using:

$$\mathbf{C}^{n+1} = \mathbf{A}^{-1} \left(\mathbf{B}\mathbf{C}^n + \Delta t \, \mathbf{Q}^n \right), \tag{3.4}$$

with appropriate boundary conditions (Neumann: $\partial c/\partial x = 0$ at $x = 0, L$) and an initial condition C^0.

This reformulation of the reaction diffusion PDE in terms of a computational linear algebra problem enables efficient solving for the oxygen concentration profile under a wide array of heat treatment conditions. By construction the CN method is stable given this stability parameter is satisfied.

$$\sigma \equiv \frac{D\Delta t}{2(\Delta x)^2}, \tag{3.5}$$

this parameter is equal to the von Neumann stability number $r = D\Delta t/(\Delta x)^2$. The Crank–Nicolson method is unconditionally stable, however, if σ is too large numerical oscillations may still occur resulting in nonphysical solutions. Therefore attention must still be given to the space and time step size to ensure numerical stability and generate a physical solution. Additionally the boundary conditions assume the concentration goes to zero at $x = L$ which means the spatial domain needs to be sufficiently large.

3.2 Computing Superconducting Properties from the Oxygen Profile

The Crank–Nicolson method allows us to simulate how oxygen diffuses into the surface of Nb during heat treatments. The main output of these simulations is the oxygen concentration profile $c(x, t)$, which tells us how much oxygen is present at different depths x inside the material. From this profile, we can calculate several important superconducting properties that influence the performance of Nb cavities and gain insight into what constitutes an optimized heat treatmnet.

3.2.1 Oxygen Concentration Profile

The oxygen concentration profile $c(x,t)$ describes the percentage of oxygen as a function of depth below the Nb surface. Heat treatments typically result in a shallow oxygen doped layer, usually no deeper than 150 nm. This layer changes the way superconducting currents are distributed in the surface region, which is critical because Nb cavities need to maintain the Meissner state to screen external magnetic fields.

3.2.2 Electron Mean Free Path ℓ

The electron mean free path ℓ is the average distance an electron can travel before scattering. When oxygen atoms are introduced during baking, they act as scattering points, reducing ℓ. There is a simple inverse relationship:

$$\ell(x) \propto \frac{1}{c(x)}. \tag{3.6}$$

Meaning that the more oxygen there is at a certain depth, the shorter the mean free path will be.

3.2.3 Effective Magnetic Penetration Depth λ_{eff}

The effective magnetic penetration depth λ_{eff} is the distance over which a magnetic field decays inside a superconductor in the Meissner state. It is used to calculate the magnetic screening profile and understand how well Nb can shield external magnetic fields.

$$\lambda_{\text{eff}}(x) = \lambda_L \sqrt{1 + \frac{\pi}{2} \cdot \frac{\xi_0}{\ell(x)}}, \tag{3.7}$$

where: λ_L is the London penetration depth, ξ_0 is the coherence length, $\ell(x)$ is the mean free path.

As more oxygen is introduced near the surface, $\ell(x)$ decreases, causing $\lambda_{\text{eff}}(x)$ to grow, affecting the distribution of supercurrents and the overall energy loss in the cavity.

3.2.4 Magnetic Field Screening Profile $B(x)$

The magnetic field profile $B(x)$ describes how an applied magnetic field penetrates into a superconductor in the Meissner state. It is important for understanding how

well the material screens magnetic fields, which directly affects energy losses and the overall performance of SRF cavities.

To calculate $B(x)$, we solve a generalized form of the London equation that accounts for the change in $\lambda_{\text{eff}}(x)$. As a result, the magnetic field profile does not follow the simple exponential decay expected for pure Nb. Instead, the decay is subtly modified by the oxygen concentration profile, influencing the superconducting properites of Nb.

3.2.5 Supercurrent Density $J(x)$

The supercurrent density $J(x)$ describes how much current is flowing at each depth to screen the magnetic field. It's proportional to the derivative of the magnetic screening profile:

$$J(x) = -\frac{1}{\mu_0}\frac{dB(x)}{dx}, \tag{3.8}$$

where μ_0 is the permeability of free space. A sharper drop in $B(x)$ near the surface means a stronger current. Because the shape of $B(x)$ depends on $\lambda_{\text{eff}}(x)$ and therefore on the oxygen profile, the supercurrent density is thereby influenced by the heat treatment.

3.2.6 Summary

From the oxygen profile $c(x)$ we calculate relevant superconducting quantities and can gain insight into how Nb behaves after heat treatments. By computing the mean free path, magnetic penetration depth, magnetic screening profile, and supercurrent density, we can directly relate a heat treatments effects to Nb cavity performance. This connection between material engineering and superconducting behavior is crucial for understanding what type of heat treatments give optimized results.

Chapter 4

Discussion and Analysis

In this chapter, we analyze the results obtained from the numerical simulations of oxygen diffusion in Nb, and examine how these results translate into changes in Nb's superconducting properties. First we look at a single heat treatment recipe — baking at 120°C for 6 hours — to investigate the resulting oxygen concentration profile and its effects on the superconducting quantities.

Then we look at the parameter space for low and mid temperature by simulating thousands of heat treatments for different time and temperature values. For each simulation, we plot three important features: (1) the peak value of the supercurrent density, (2) the supercurrent density at the surface, and (3) the depth at which the peak occurs. These results provide insight into how different baking conditions influence superconducting performance and can help quantify the effectiveness of a given recipe.

4.1 Understanding the Effects for a Given Recipe

Figure 4.1 shows the results of a numerical simulation for a 120°C, 6-hour baking recipe. The oxygen concentration profile (top panel) shows a sharp drop in the first ∼20 nm of the Nb, followed by a long tail going to zero in the bulk. This is shape is desired as it mimics the effects of an SS-bilayer and reduces the electron mean free path $\ell(x)$ near the surface, which in turn increases the effective magnetic penetration depth $\lambda_{\text{eff}}(x)$ in that region.

Although the resulting magnetic field screening profile $B(x)$ only shows a subtle deviation from the exponential decay expected for pure Nb, the effect on the super-

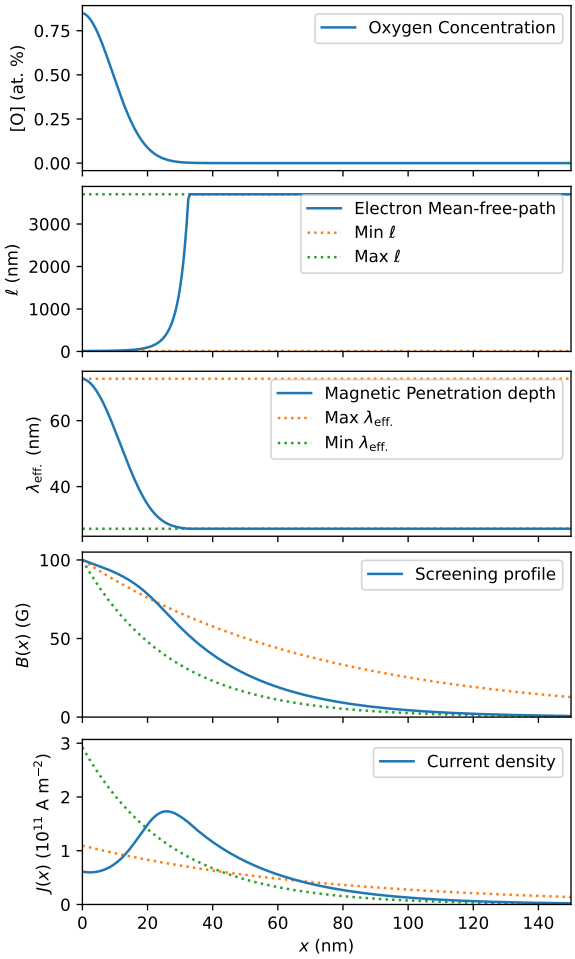

Figure 4.1: Effect on superconducting properties for Baking Conditions: 6 h,120°C

current density $J(x)$ is much more significant. This is because $J(x)$ is proportional to the derivative of $B(x)$, so even small changes in the slope of $B(x)$ produce noticeable shifts in the shape and distribution of the screening current.

The important thing to notice is that the peak of $J(x)$ is pushed deeper into the material, and the surface value of the supercurrent density is reduced. This shift in the supercurrent deeper into the material is beneficial for Nb cavity performance because it helps reduce energy loss at the surface. By adjusting the oxygen profile through baking, we can improve how the cavity behaves with stronger RF fields applied and stop the cavity quality factor from dropping off.

4.2 Searching for an Optimized Recipe

To better understand how different heat treatment parameters affect SRF cavity performance, we simulated thousands of unique baking recipes across a broad range of time and temperature combinations. For each simulation we plotted superconducting quantities such as the peak value of the supercurrent density $J(x)$, the value of $J(x)$ at the surface, and the depth at which the peak occurs. These metrics provide insights into how the superconducting properties change with varying oxygen concentration profiles.

Below in figure 4.2 we can see the value of the peak supercurrent normalized by the peak in clean Nb. There are two distinctive 'bands' of contour lines corresponding to sets of potentially optimized recipes.

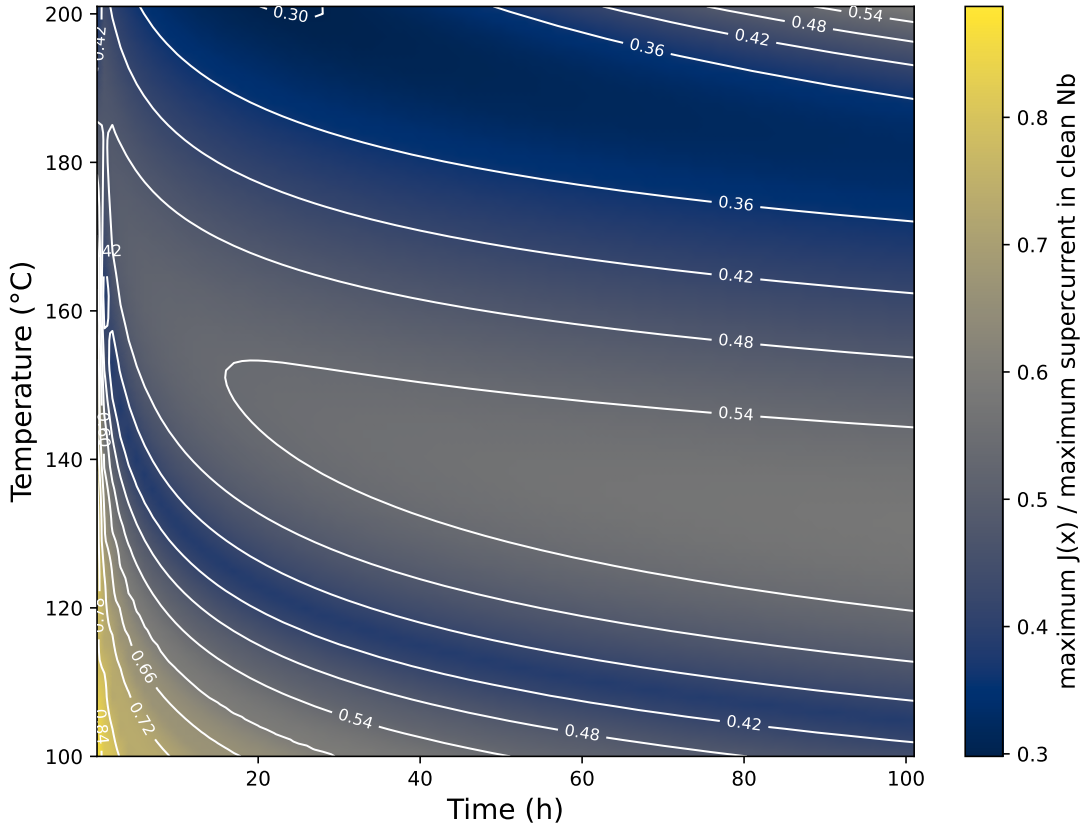

Figure 4.2: Peak Supercurrent Density Variation with Baking Conditions

To understand what superconducting properties correspond to the best recipe, its crucial to note that no single metric can determine whether a recipe is optimal. For

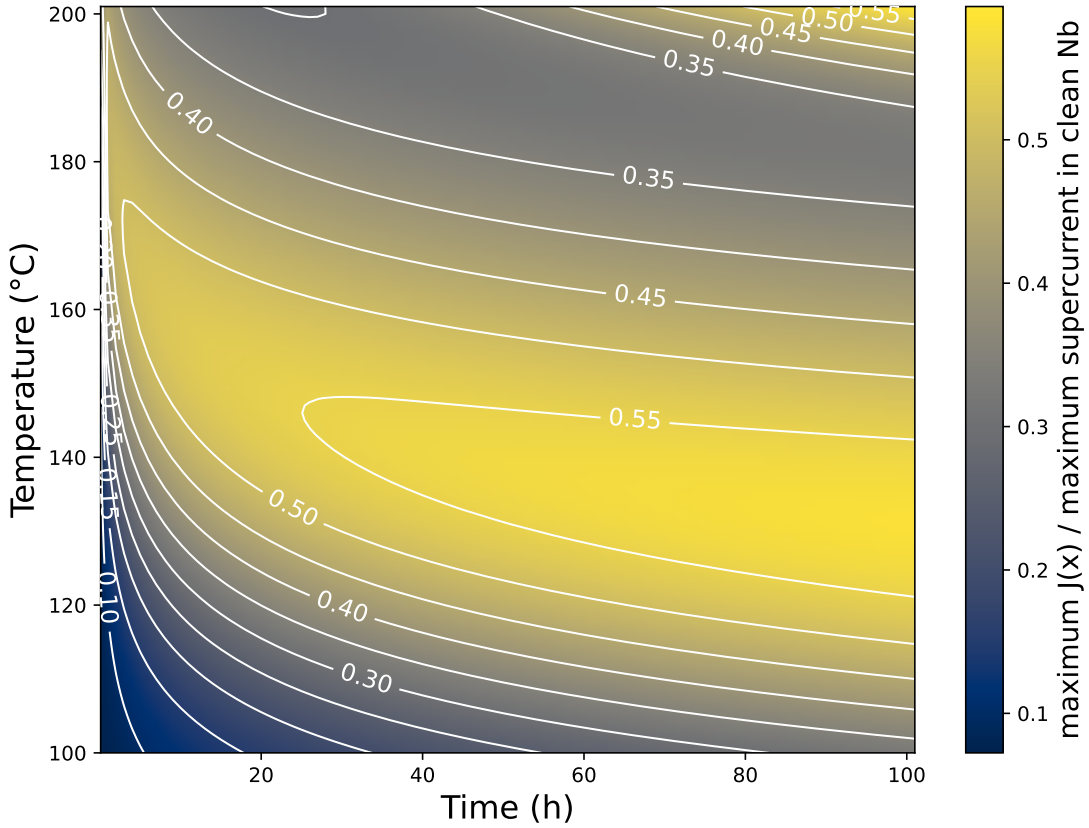

Figure 4.3: Surface Supercurrent Density Variation with Baking Conditions

example, if we focused only on minimizing the peak supercurrent density without considering its depth, we might choose a recipe of 200°C, 40-hours where in figure 4.2 we can clearly see a minimized peak. While this might appear optimal, to the contrary it would not give us even close to the effects we want, as by comparing with figure 4.4 we can see this recipe corresponds to a peak that occurs right at the surface of the Nb sample. If the peak supercurrent density occurs at the surface, it indicates that the superconducting properties of Nb have been destroyed. Meaning, the material no longer effectively screens magnetic flux, resulting in increased energy losses and worse cavity performance.

This clearly demonstrates why it is essential to evaluate multiple metrics when searching for an optimized recipe. A good heat treatment should not only reduce the peak and surface values of $J(x)$ but also push the current peak away from the surface and into the bulk, such that the Nb can maintain a meissner state and properly screen magnetic flux.

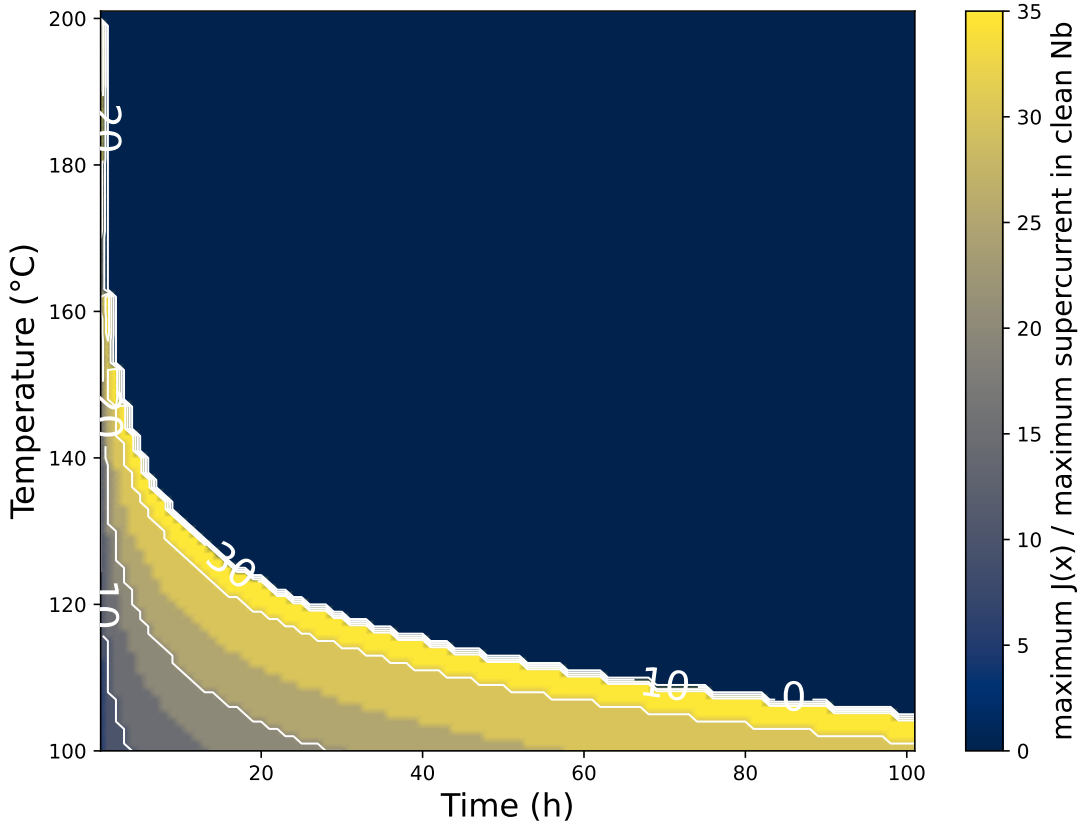

Figure 4.4: Depth of Peak Supercurrent Variation with Baking Conditions

Taking these various metrics into account, we can see a clear contour corresponding to a minimized peak supercurrent while having that peak pushed into the bulk and at the same time minimizing the surface supercurrent value. This demonstrates not only how we can start to understand what constitutes an optimized recipe but also how in such an optimization problem where you are looking at multiple metrics you necessarily have to make tradeoffs to get an optimal solution.

Additionally a key takeaway comes from analyzing the position of the supercurrent peak, we see a clear boundary beyond which the superconducting behavior is effectively destroyed. Recipes that exceed a certain time or temperature threshold result in the supercurrent occurring right at the surface, indicating that too much oxygen has been dissolved into the sample. This sets a theoretical limit on the treatment parameters, beyond which we not only don't see further optimization of Nb's superconducting properties, we also see them effectively destroyed. This emphasizes the importance of precise recipes and baking mechanisms to push Nb superconducting

qualities as far as possible without going past this limit.

Chapter 5

Conclusions

This project explored how baking niobium SRF cavities under different conditions affects their superconducting performance. By simulating the diffusion of oxygen into Nb during heat treatments, we were able to study how the resulting oxygen profiles change important superconducting properties like magnetic field screening and supercurrent distribution.

We showed through analyzing one specific recipe: baking at 120°C for 6 hours that these type of heat treatments can create an oxygen concentration near the surface of the material, with a steep drop-off into the bulk. This type of profile is beneficial because it causes the supercurrent to shift away from the surface and deeper into the material, reducing surface losses and helping the cavity maintain good performance at high RF fields.

Next we simulated thousands of recipes across a wide range of time and temperature combinations. For each one, we looked at three key metrics: the peak supercurrent value, the value at the surface, and the depth at which the peak supercurrent occurs. These metrics enabled a greater understanding of what makes a recipe optimized and set the foundation for rigorously defining a figure of merit to quantify a given recipe.

We found it was important to consider all metrics in the analysis. If only the peak supercurrent was looked at then incorrect conclusions were made as to what baking conditions gave an optimized recipe. Some recipes that minimize the peak actually cause it to occur at the surface, which doesn't give us the superconducting properites we desire. Instead, the best recipes are the ones that keep the peak low, keep the surface supercurrent low, and also push the peak deeper into the bulk of Nb.

Notably, we found a clear limit for baking temperature and time, beyond which

the peak supercurrent always occurs right at the surface, making it impossible to achieve an optimized result.

Chapter 6

Future Work

While this project has provided insights into how baking affects the superconducting properties of niobium SRF cavities, there is still much more to be done to fully understand and define what makes an optimized heat treatment recipe.

The numerical approach and codebase developed offer a solid foundation for future research. By simulating how oxygen diffuses into Nb and how this affects its superconducting quantities, we now have software that can explore the parameter space of baking conditions.

One important direction for future work is to improve the accuracy of the numerical method. In particular, the current simulations assume a constant diffusion coefficient, but at higher temperatures it becomes relevant to consider a time dependent diffusion coefficient.

Another interesting direction is multi-step heat treatments. For example, after an initial heat treatment the sample could be exposed to air again and re-baked to further modify the doping profile. Simulating these more complex treatment sequences could lead to new ways of engineering the surface properties of Nb cavities.

In addition, while this project focused on three main metrics — peak supercurrent, surface supercurrent, and peak supercurrent depth — they still need to be combined into a quantitative figure of merit. Defining such a figure could help systematically compare different recipes and identify optimal regions of the parameter (recipe) space.

Overall, this project demonstrates the value of a numerical approach in understanding and optimizing Nb cavity treatments. Future work would enable the discovery of better recipes, a more complete theoretical understanding of cavity performance, and more efficient cavity production.

Appendix A

Crank Nicolson Solver

```
"""Crank-Nicolson example.

Adapted from: https://georg.io/2013/12/03/Crank_Nicolson

see also: https://math.stackexchange.com/a/3311598
"""

class CNSolver:
    """Crank-Nicolson Solver for 1D Diffusion Problems.

    This class encapsulates the Crank-Nicolson method to solve diffusion equations
    in 1D with specified initial and boundary conditions.

    Attributes:
        D_u (float): Diffusion coefficient (in nm^2/s).
        u_0 (float): Initial concentration close to x = 0 (e.g., at. % nm).
        v_0 (float): Background concentration (e.g., at. % nm).
        t_h (float): Maximum time in hours.
        N_x (int): Number of spatial grid points.
        x_max (float): Maximum spatial boundary (nm).
        N_t (int): Number of time grid points.
        x_grid (np.ndarray): Spatial grid.
```

```
23          t_grid (np.ndarray): Temporal grid.
24          sigma_u (float): Proportionality term for Crank-
               Nicolson.
25      """
26
27      def __init__(self, T, u_0=1e3, v_0=1e1, t_h=48, x_max
           =500.0, N_x=1001, N_t=4001):
28          self.T = T
29          self.u_0 = u_0
30          self.v_0 = v_0
31          self.t_h = t_h
32          self.x_max = x_max
33          self.N_x = N_x
34          self.N_t = N_t
35
36          # Constants
37          self.D_u = D(T)  # Diffusion coefficient (in nm^2/s)
38          self.c_0 = v_0 + u_0  # Initial concentration
39
40          # Spatial and temporal grids
41          self.x_grid = np.linspace(0.0, x_max, N_x, dtype=np.
               double)
42          self.dx = np.diff(self.x_grid)[0]
43
44          self.s_per_h = 60.0 * 60.0
45          self.t_max = t_h * self.s_per_h
46          self.t_grid = np.linspace(0.0, self.t_max, N_t, dtype=
               np.double)
47          self.dt = np.diff(self.t_grid)[0]
48
49          # Stability parameter
50          self.r = (self.D_u * self.dt) / (self.dx * self.dx)
51          self.stability = "STABLE" if self.r <= 0.5 else "
               POTENTIAL OSCILLATIONS"
52
53          # Crank-Nicolson proportionality term
54          self.sigma = 0.5 * self.r
```

```
55
56
57      def gen_sparse_matrices(self):
58          """Generate the sparse matrices "A" and "B" used by
                the Crank-Nicolson method.
59
60          Args:
61              N_x: Dimension of (square) matrices.
62              sigma: The "nudging" parameter.
63
64          Returns:
65              The (sparse) matrices A and B.
66          """
67
68          # common sparse matrix parameters
69          _offsets = [1, 0, -1]
70          _shape = (self.N_x, self.N_x)
71          _format = "csr"
72
73          # define matrix A's elements
74          _A_upper = [-self.sigma]
75          _A_diag = [1 + self.sigma] + [1 + 2 * self.sigma] * (
                self.N_x - 2) + [1 + self.sigma]
76          _A_lower = [-self.sigma]
77          _A_elements = [_A_upper, _A_diag, _A_lower]
78
79          # create matrix A
80          _A = sparse.diags_array(
81              _A_elements,
82              offsets=_offsets,
83              shape=_shape,
84              format=_format,
85          )
86
87          # define matrix B's elements
88          _B_upper = [self.sigma]
```

```
89          _B_diag = [1 - self.sigma] + [1 - 2 * self.sigma] * (
               self.N_x - 2) + [1 - self.sigma]
90          _B_lower = [self.sigma]
91          _B_elements = [_B_upper, _B_diag, _B_lower]
92
93          # create matrix A
94          _B = sparse.diags_array(
95              _B_elements,
96              offsets=_offsets,
97              shape=(self.N_x, self.N_x),
98              format=_format,
99          )
100
101         # return both matrix A and B
102         return _A, _B
103
104     def get_oxygen_profile(self):
105         """Solve the diffusion equation using the Crank-
               Nicolson method.
106
107         Returns:
108             np.ndarray: The solution record (time x space).
109         """
110         # Initial condition: Concentration is all in the first
               spatial bin
111         U_initial = sparse.csr_array([self.v_0 / self.dx] +
               [0] * (self.N_x - 1))
112         U_record = np.zeros((self.N_t, self.N_x), dtype=np.
               double)
113
114         for i, t in enumerate(self.t_grid):
115             if i == 0:
116                 # Record the initial condition
117                 U_record[i] = U_initial.toarray()
118             else:
119                 # Source term (plane source at x = 0)
```

```
120                 f_vec = sparse.csr_array([q(t, self.T) * (self
                        .dt / self.dx)] + [0] * (self.N_x - 1))
121
122                 # Generate matrices (could be precomputed if
                        D_u is constant)
123                 A, B = self.gen_sparse_matrices()
124
125                 # Solve for the next time step
126                 U = sparse.csr_array(U_record[i - 1])
127                 U_new = sparse.linalg.spsolve(A, B @ U + f_vec
                        )
128                 U_record[i] = U_new
129
130         return U_record
```

Listing A.1: Crank–Nicolson Solver Class for 1D Oxygen Diffusion

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