Defect Profile Engineering in Niobium for Particle Accelerator Applications

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Introduction & Motivation

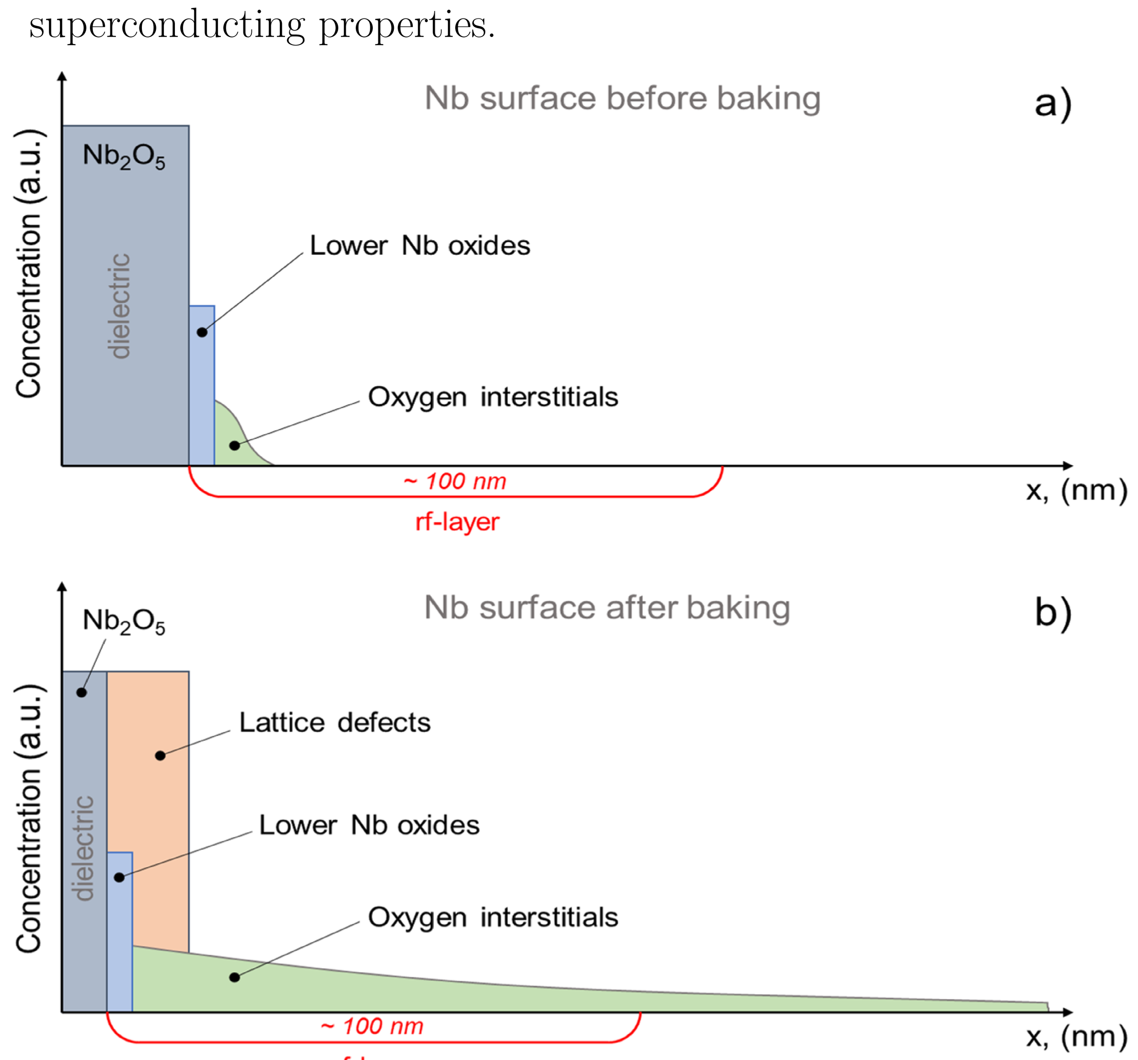
- **Superconducting radio-frequency (SRF) cavities**, made from **niobium (Nb)**, are critical components in particle accelerators, transforming stored electromagnetic energy into kinetic energy of charged particles.
- **Heat treatments** in a vacuum induces oxygen doping in the near-surface region (~5 nm), modifying Nb's superconducting properties.
- By tailoring the oxygen concentration profile through theoretical simulations, cavity performance may be improved beyond current empirical methods.
- **The standard recipe** is 120°C for 48hrs increasing the accelerating voltage by roughly a factor of 2.
- This work employs **numerical methods** to solve the reaction-diffusion equation and explore optimal treatment conditions.

Surface Oxide Dissolution and Diffusion

- The dissolution of niobium's surface oxide involves a sequence of **reduction reactions:**

$$\begin{aligned} Nb_2O_5 &\xrightarrow{k_1} 2NbO_2 + O, \\ NbO_2 &\xrightarrow{k_2} NbO + O, \\ NbO &\xrightarrow{k_3} Nb + O, \end{aligned} \tag{1}$$

where k_i is the reaction rate constant.
- **The baking process** reduces the higher Nb oxides, releasing oxygen as interstitial impurities, whose presence affects Nb's superconducting properties.



- This production of oxygen and its diffusion into Nb is captured by the reaction-diffusion equation:

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

where $c(x,t)$ is the oxygen concentration, $D(T(t))$ is the diffusion coefficient, $q(t,T(t))$ is the rate of oxygen production and T is the absolute temperature.

Solving the Reaction Diffusion Equation

- **Numerical Solution via the Crank-Nicolson (CN) Method:** Due to the lack of a general analytical solution, we employ CN method to discretize the reaction/diffusion problem, creating a system of linear equations solved at each time step.
- **Crank-Nicolson Method:** By approximating the derivatives in equation (2) and encoding the oxygen diffusion effects into matrices we can write the system of linear equations as:

$$\mathsf{A}\mathbf{C}^{n_{t+1}} = \mathsf{B}\mathbf{C}^{n_t} + \Delta t \mathbf{Q}^{n_t}, \tag{3}$$

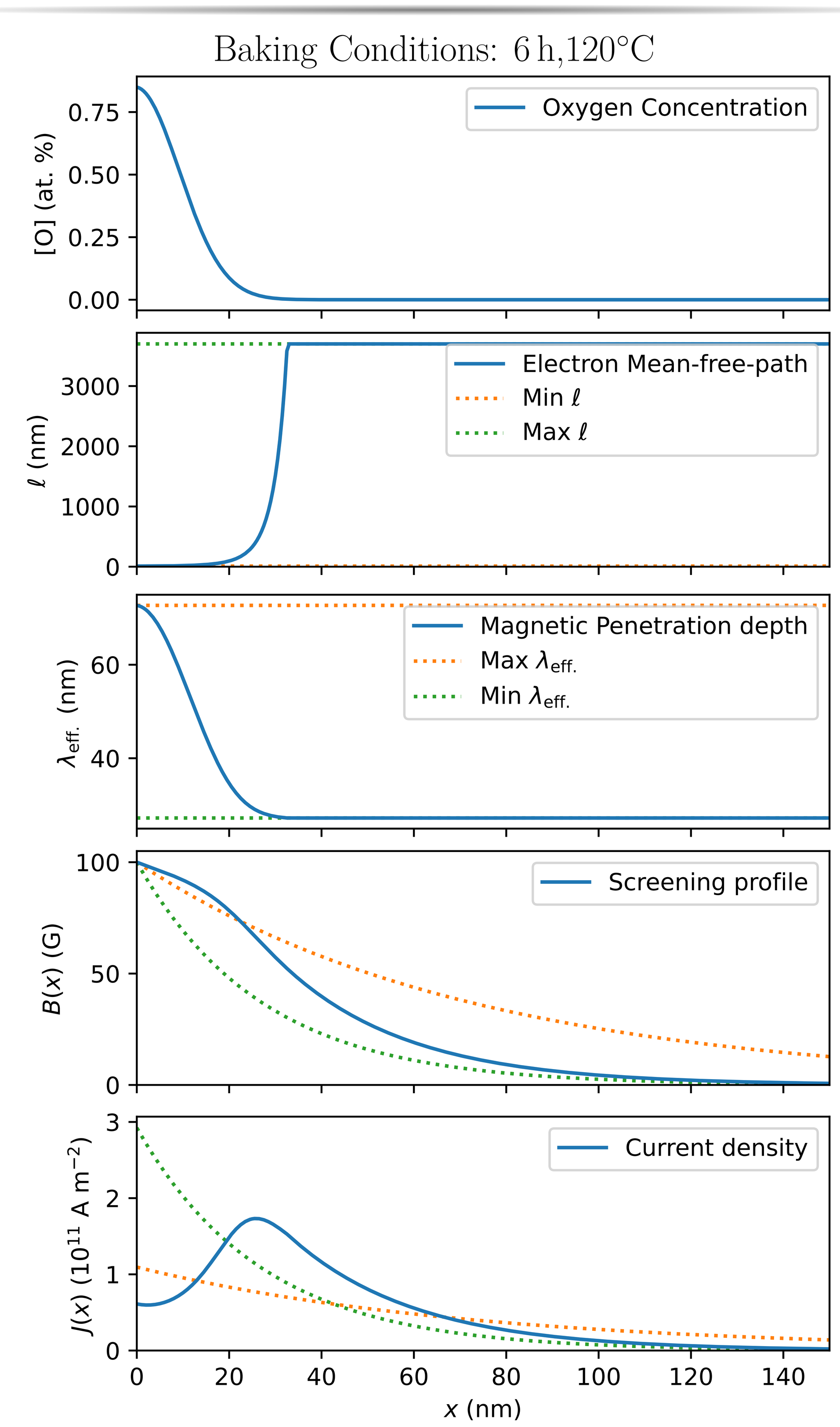
where $\mathbf{C}^i$ is the concentration vector, A and B are tridiagonal matrices defining the spread of oxygen from one spatial grid to the next. Δt is the time step, and $\mathbf{Q}^i$ is the source term.
- **Efficient Computation:** This system can be directly solved through standard computational linear algebra techniques.

Connection to Accelerator Cavities

- **Fine-Tuning Nb superconducting properties:** by introducing oxygen interstitials we reduce the electron mean free path thereby increasing the magnetic penetration depth and hence modifying the magnetic screening profile which affects the shape supercurrent density distribution.
- **Inhomogeneous doping** shifts the peak supercurrent further into the clean bulk of Nb, optimizing cavity performance.
- **Minimizing Energy Dissipation:** an optimal treatment reduces the surface supercurrent density while pushing the peak current to a maximum depth.

Simulation Results

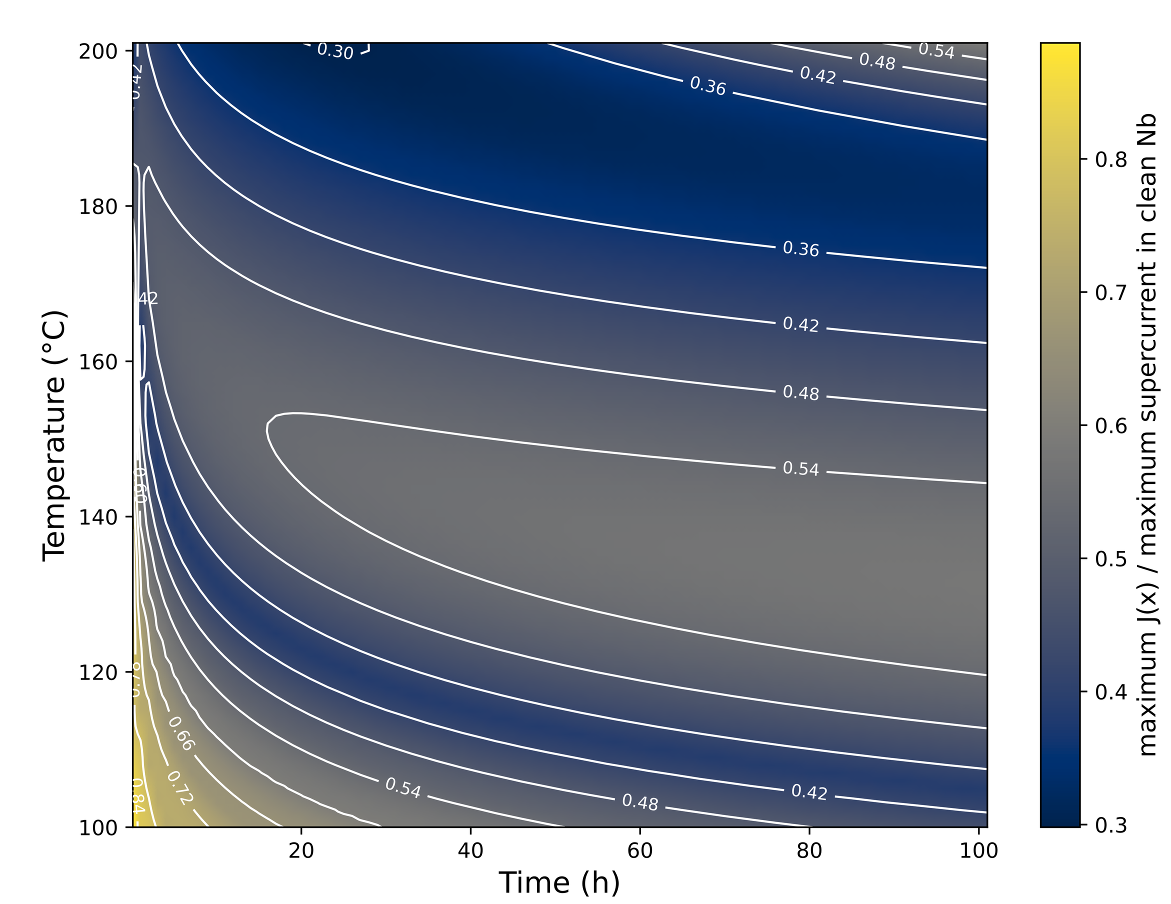
Effect of Oxygen Diffusion on Superconducting Properties



- **Oxygen Concentration Profile:** Displays the percent oxygen as a function of depth x in niobium. Shallow oxygen impurity profiles resulting from heat treatments can deform the spatial distribution of supercurrents.

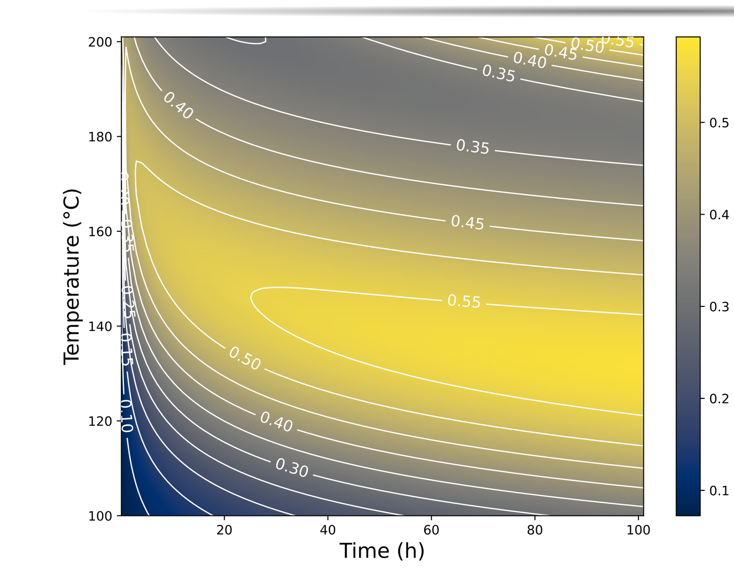
- **Electron Mean Free Path ℓ:** represents the average distance an electron travels before it experiences a scattering event with an impurity. In ultra-clean Nb, ℓ continues to increase asymptotically and can become extremely large in the absence of impurities and defects.
- **Effective Magnetic Penetration Depth λ_{eff}:** the characteristic length over which external magnetic flux is screened below a (Meissner state) superconductor's surface.
- **Magnetic Field Screening Profile $\mathbf{B(x)}$:** the spatial decay of magnetic flux below a (Meissner state) superconductor's surface.
- **Supercurrent Density $\mathbf{J(x)}$:** density of superconducting electrical currents that screen magnetic flux.

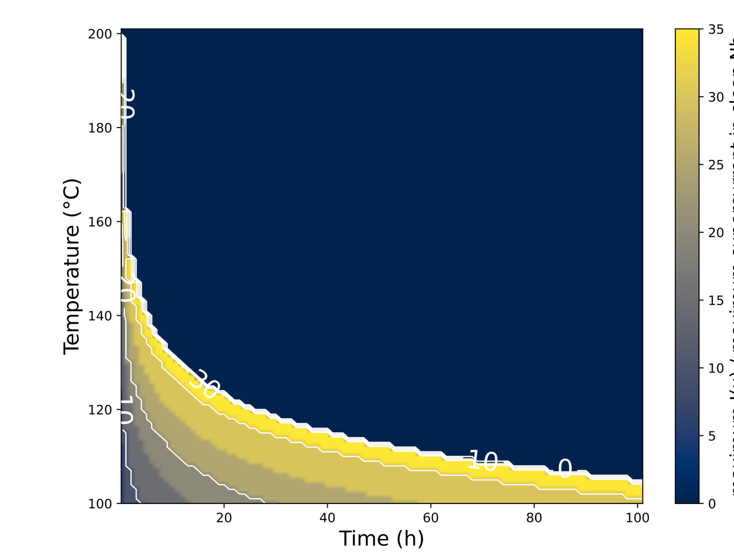
How the Peak Supercurrent Density Varies with Baking Conditions



- **Optimized Treatments:** By running the simulations thousands of times for different baking conditions we see a distinct "valley" indicating a minimized peak supercurrent density.

Surface Supercurrent Density and Peak Supercurrent Position





- We look at the surface current density as another variable to try and gain insight into the cavity optimizations. We see similar distribution of contour lines as compared to the peak supercurrent density.
- We see a sharp drop off of the maximum peak supercurrent following the "valley" shape of the previous graphs, a rather unintuitive result showing how too high a temperature or baking time flattens the supercurrent distribution.

Conclusions

- **Simulations:** Theoretical simulations of heat treatment recipes give novel insights into the nuances of the treatment effects, specifically how through chemical transformations we can engineer the oxygen defect profile to affect the supercurrent density.
- **Ideal Conditions:** The results suggest that low baking temperatures < 120°C of moderate duration minimize supercurrents near the surface, but with a density that "peak" as far below the surface as possible.
- **Future work:** Quantifying "recipe" performance by combining peak supercurrent, surface supercurrent, x position of peak current and more to develop a figure of merit for Nb SRF cavity heat treatments.
- Explore how multiple heat treatments, where Nb is exposed to air after baking, thereby re-oxidizing the sample giving it a new oxide surface layer and then baking again could lead to new defect profile engineering possibilities.

References

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[5] Image Credit: Department of Energy's Thomas Jefferson National Accelerator Facility (Jefferson Lab).