Fermi National Accelerator Laboratory

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Characterizing the Dirty Layer in Superconducting RF Cavities

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Acknowledgements

Abstract

RF cavities are devices used to accelerate charged particles in accelerators by creating a resonant electromagnetic field in the radio-frequency range. The enriched impurity or "dirty" layer found on the surface of high gradient cavities was investigated since theoretical models show that tuning the thickness of this impurity layer can lead to enhancements in accelerating gradient. Experimental data from Vertical cavity testing was processed and fit using Bardeen Cooper Schrieffer(BCS) theory to find mean free path. This data is then analyzed using a theoretical model to identify the limiting factors of present day cavities to find that they are not limited by the thickness of the dirty layer.

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List of Variable and Constant definitions

Symbol	Description
π	3.14159265358979323846
μ_0	Vacuum Permeability ($4\pi * 10^7$ H/m)
ξ	Coherence Length
C_s	Concentration at the surface
T_c	Critical Temperature
D	Diffusion Constant
$\lambda_{\text{coupling}}$	Electron-phonon coupling parameter
f	Frequency
g	Geometric factor (here: 270Ω)
κ	Ginzburg-Landau Parameter ($\frac{\lambda}{\xi}$)
λ	Penetration depth
B_s	Superheating Field
T	Temperature of superconductor
B_{crit}	Thermodynamic Critical Field
d	Thickness of Dirty Layer
t	Time
A	Vector Potential

Chapter 1

Introduction

Superconducting cavities made from niobium are used in most high-energy accelerators due to their greatly reduced power consumption and ability to generate very high accelerating gradients of the order of 45 MV/m.

Cavity performance is intimately related to the material properties (e.g. impurity content) in the first $\sim$ 100 nm from the RF surface. Advanced material characterizations showed that cavities able to reach high gradients (namely 120°C baked[1] and N-infused cavities[2]) possess an enriched impurity or dirty layer on the surface with thickness comparable or smaller than the penetration depth[3] ($\sim$ 40 nm for Nb), as opposed to cavities that are limited to lower gradients (N-doped[4] and electropolished[1] cavities) which instead show constant impurity profile inside the penetration depth.

Theoretical investigations on the effect of such a dirty layer on the cavity performance[5] suggest that the accelerating gradient is enhanced if the impurity content and thickness of the layer are tuned properly.

Several cavities that were Infused with Nitrogen for different time periods were studied and the results were used to simulate what the optimal fields of such processes should be in order to understand what is limiting the maximum quench field attainable in the cavity.

1.1 Cavity Processing

During fabrication, cavities undergo different processes that enhance their accelerating gradient. The cavities being studied here are all Nitrogen infused.

1.1.1 Nitrogen Infusion

N-infusion is a treatment that modifies the first $\sim$ 100 nm near the surface by adding interstitial Nitrogen. The standard N-infusion thermal treatment is composed of two steps:

- Cavities are treated for 3 hours at 800°C in High Vacuum

- Nitrogen is then injected at the temperature of 120°C for a time period ranging in between 24 hours to 90 hours.

No chemistry is needed after the treatment.

1.2 Theory

1.2.1 Bardeen Cooper Schrieffer(BCS) Theory

This was the first microscopic theory of superconductivity. It uses electron-phonon interactions to explain formation of cooper(electron) pairs that follow Bose-Einstein statistics. The phonon exchange interaction allows for an attractive potential between electrons which causes them to pair up.

BCS theory does not allow for strong coupling (Assumes $\lambda_{coupling} << 1$), i.e the effects of electrons on the phonons themselves are not considered, which makes it a crude approximation for materials like Niobium. This is partially overcome by arbitrarily adjusting coherence length and penetration depths to scale and accommodate these effects[6]. For this study BCS theory is used as a fitting module in order to extract parameters like mean free path from experimentally identifiable characteristics of the superconducting cavity.

1.2.2 Kubo's Model

Takayuki Kubo developed a model for finding the maximum attainable quench field using an Superconductor-Superconducting substrate structure. The S-S model mimics the surface of a superconductor that consists of superconductors with different penetration depths.[5]
Niobium surface after the Nitrogen infusion has a depth dependent mean-free path and hence a depth dependent penetration depth. This can be described by an S-S bilayer with a thin dirty Nb and a clean Nb substrate as the simplest model.
The current and field distribution is obtained by solving the London equation(equation 1.1) with $\lambda = \lambda_1$ for $0 \le x \le d$ and $\lambda = \lambda_2$ for $x \ge d$

$$\lambda^2 A'' - A = 0 \tag{1.1}$$

Figure 1.1: S-S model

This model is built in the London limit and due to these assumptions it is not expected to have a quantitative agreement with experimental data but the trend that is followed should give insight into the limitations of the cavity.

Chapter 2

Experimental Data Collection

2.1 Vertical Cavity Testing

Nitrogen infused cavities prepared at the same temperature but different infusion duration were tested at the Vertical Test Facility to record their response to RF signal under different conditions. The following table lists the cavities that were studied:

Cavity Name	Nitrogen Infusion Duration	Frequency vs Temperature data
AES018	24 hours	✗
PAV007	48 hours	✗
AES015	48 hours	✗
PAV012	48 hours	✓
AES010	48 hours	✗
AES015	48 hours	✗
RI002	60 hours	✗
RI001	60 hours	✓
AES021	60 hours	✓
RI006	90 hours	✓
RI003	90 hours	✗

The cavities for which frequency vs temperature data is available were used for BCS fitting to find out the average mean free paths for theoretical model.
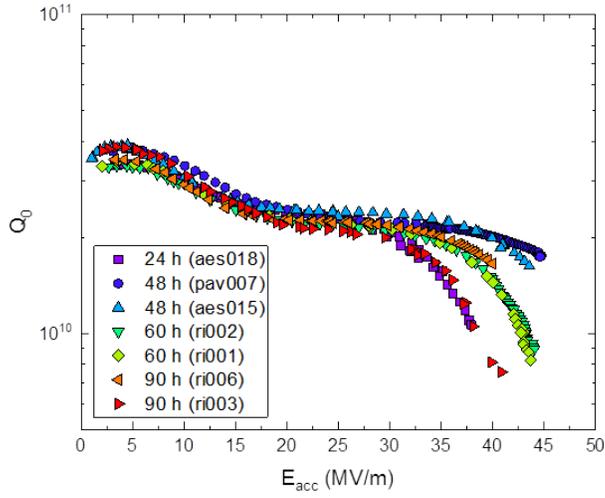
Figure 2.1: Quality factor measurements across different RF field strengths

The Qualiy factor curve gives a good idea about the accelerating capabilty of the cavity. Not all the cavities are shown for the sake of clarity.
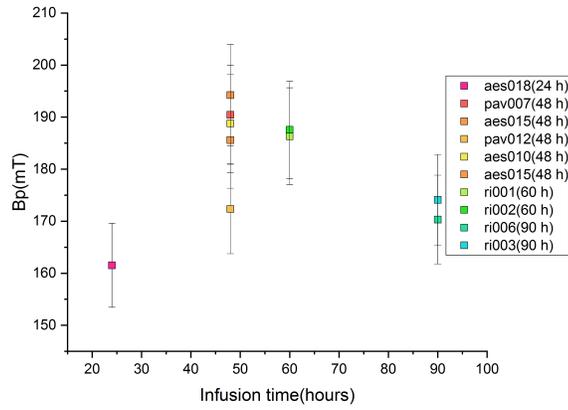
Figure 2.2: Quench field for treatments at different temperatures

The maximum magnetic field the cavity was able to hold before quenching is noted since according to Kubo's Model(Section 1.2), it should depend on the thickness of the dirty layer.

Chapter 3

Data and Simulation Analysis

3.1   BCS Fitting

The Frequency-Temperature dependence data is processed and fit using a python program using the Halbriter program in C(Appendix A). The program allowed for easy handling of a large number of datasets and created a $\sim 4800\%$ increase in computational speed.

The data processing consists of correcting for the errors due to pressure deviations in the frequency data, removing outliers and interpolating to get a fixed number of points for the fit.

The fit is performed in multiple steps to find the various parameters to a small uncertainity(details in Appendix A).
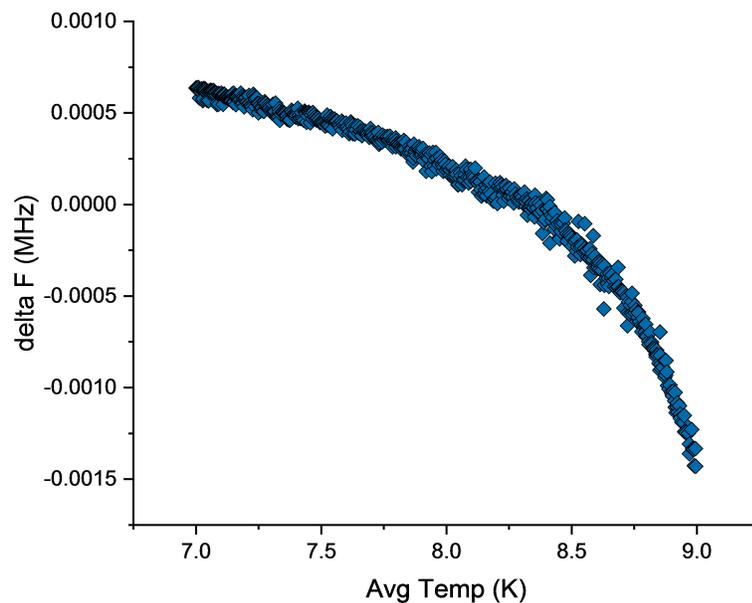
Figure 3.1: Change in frequency(pressure corrected) with temperature

The frequency(fig 3.1) is transformed into penetration depth by equation 3.1 after correcting for pressure variations

$$\Delta\lambda = -\frac{g\Delta f}{\mu_0 \pi f_0^2} \tag{3.1}$$

The transformed data across different temperature scales is fit(fig: 3.2) to get the mean free path for each bin of data.
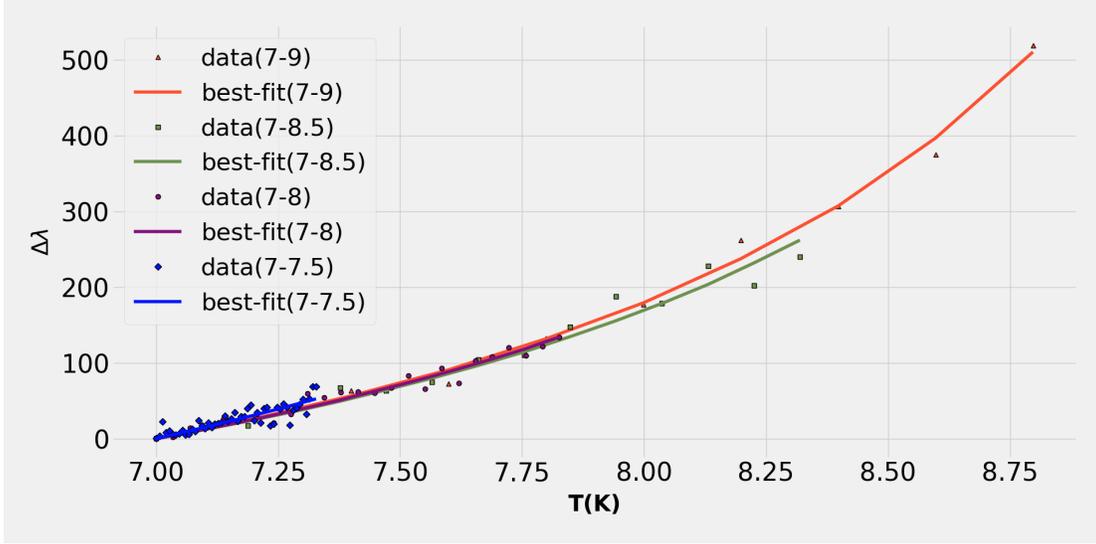
Figure 3.2: BCS fits for different temperature sets

The different temperatures allows us to probe at different depths by using equation 3.2.

$$\frac{\lambda(T)}{\lambda_0} = \frac{1}{\sqrt{1 + \left(\frac{T}{T_c}\right)^4}} \tag{3.2}$$

This means that the fits for lower temperature gives us the average mean free path at shallow depths while that spanning a large temperature range will give the average mean free path across a large depth.

Plotting the mean free paths across different depths found through BCS fitting (fig:3.3) shows the expected trend of it increasing with depth. However, the dip towards greater depths is curious and requires further exploration,
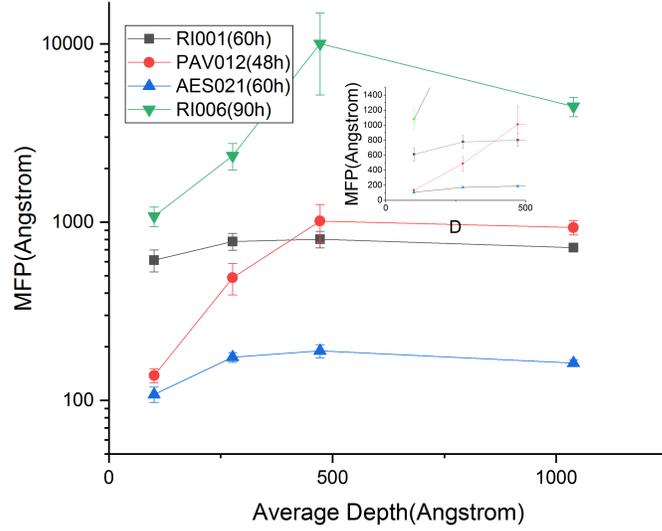
Figure 3.3: Average mean free path across different depths

Correlating the shallow depth mean free paths with the maximum field(fig: 3.4) that the cavity experiences shows no particular trend but the values agree with the expected range.
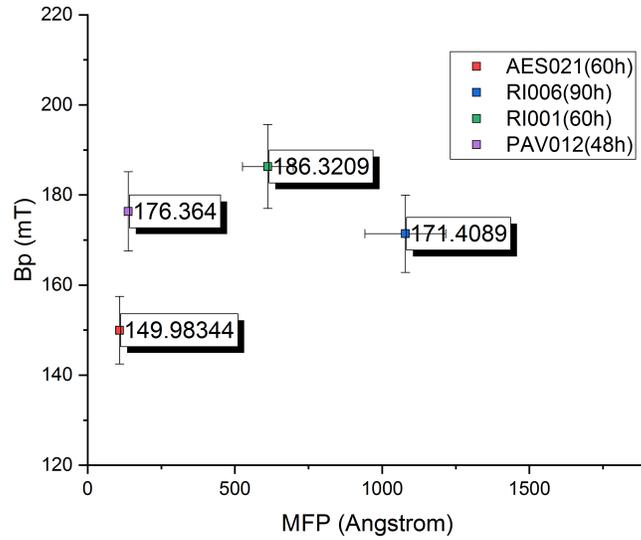
Figure 3.4: Quench field for for cavities with Dirty layer mean free path

The shallow depth mean free paths across several cavities are averaged as the mean free path of the dirty layer in theoretical simulation.

3.2 Diffusion Analysis

To find what the depth of the dirty layer should be Nitrogen concentration profile was used.

The SIMS[1] data for a 48 hour Nitrogen infused cavity was used to find out the diffusion constant(fig: 3.5) for Nitrogen in Niobium using Fick's law solution(equation 3.3) for diffusion with constant surface concentration[7].

$$C = C_s \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{3.3}$$
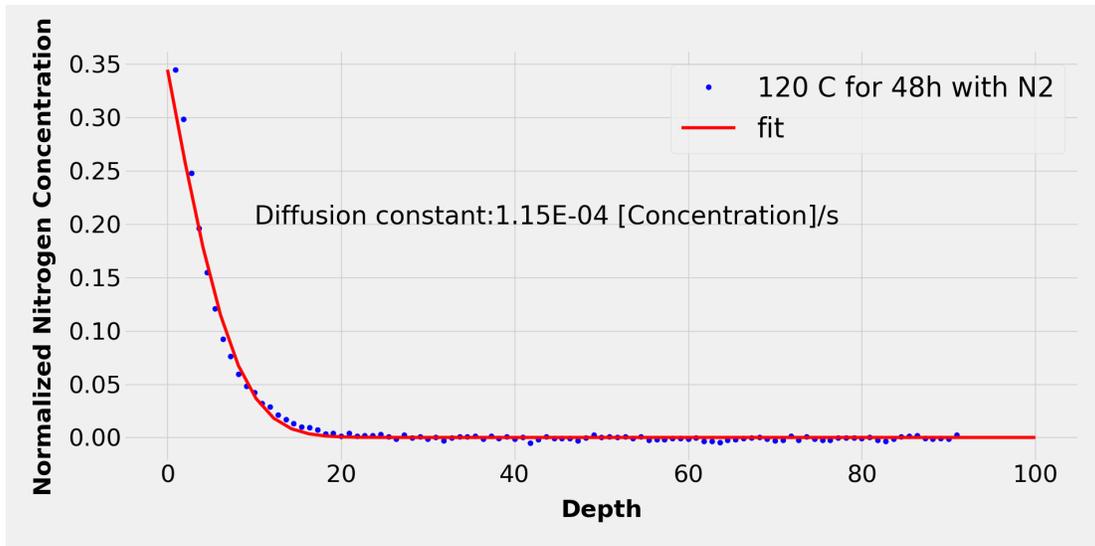
Figure 3.5: Fitting Nitrogen concentration data using Fick's Law

The diffusion constant should theoretically remain the same for a given set of materials at a given temperature[7].

The diffusion constant thus found is then used to simulate the concentration profile for the other timescales of interest, namely, 24, 48, 60, and 90 hours(fig: 3.6).

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[1]Secondary-ion mass spectrometry (SIMS) is a technique used to analyze the composition of solid surfaces and thin films by sputtering the surface of the specimen with a focused primary ion beam and collecting and analyzing ejected secondary ions.
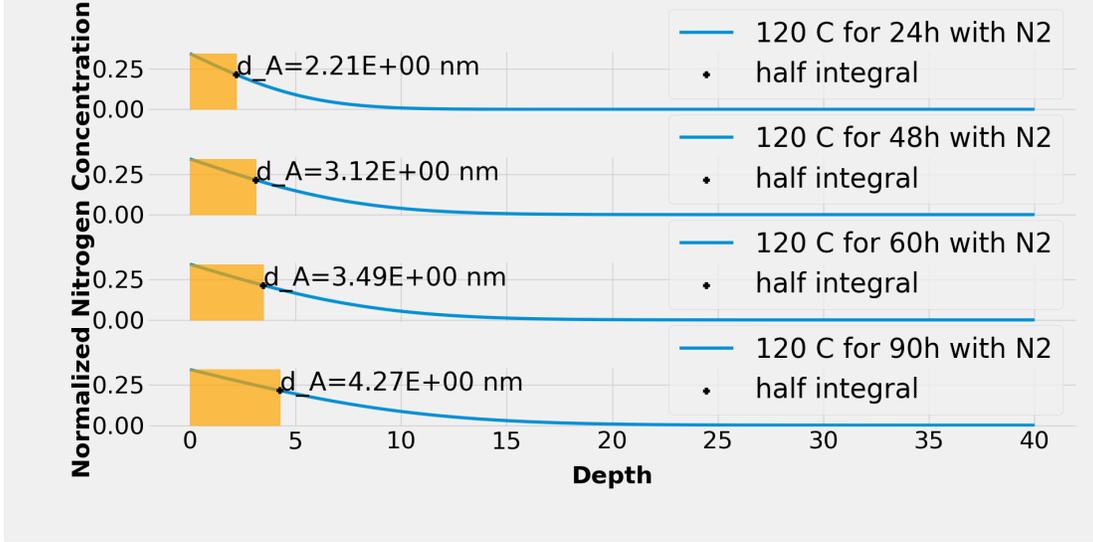
Figure 3.6: Simulating for other time scales using parameters from fit

The depth that splits the Nitrogen concentration equally is noted as the depth of the dirty layer.

3.3   Simulating theoretical model

The depth and mean free path data acquired are then used to build a simulation of Kubo's Model.

The superheating field[2] is found within Ginzburg-Landau Theory [8] using equation 3.4

$$\frac{B_s(\kappa)}{\sqrt{2}B_{crit}} \approx \frac{\sqrt{10}}{6} + \frac{0.3852}{\sqrt{\kappa}} \tag{3.4}$$

The Maximum field in Kubo's Model is given by equation 3.5 where γ_1 and γ_2 are given by equations 3.6 and 3.7 respectively.

$$B_{max} = \min\{\gamma_1^{-1}B_s^{(\text{Dirty Layer})}, \gamma_2^{-1}B_s^{(\text{Substrate})}\} \tag{3.5}$$

$$\gamma_1 = \frac{\sinh\frac{d}{\lambda_1} + \frac{\lambda_2}{\lambda_1}\cosh\frac{d}{\lambda_1}}{\cosh\frac{d}{\lambda_1} + \frac{\lambda_2}{\lambda_1}\sinh\frac{d}{\lambda_1}} \tag{3.6}$$

$$\gamma_1 = \frac{d}{\cosh\frac{d}{\lambda_1} + \frac{\lambda_2}{\lambda_1}\sinh\frac{d}{\lambda_1}} \tag{3.7}$$

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[2]a metastable state which sets the upper limit of sustainable magnetic fields on the surface of a superconductors before flux starts to penetrate into the material.
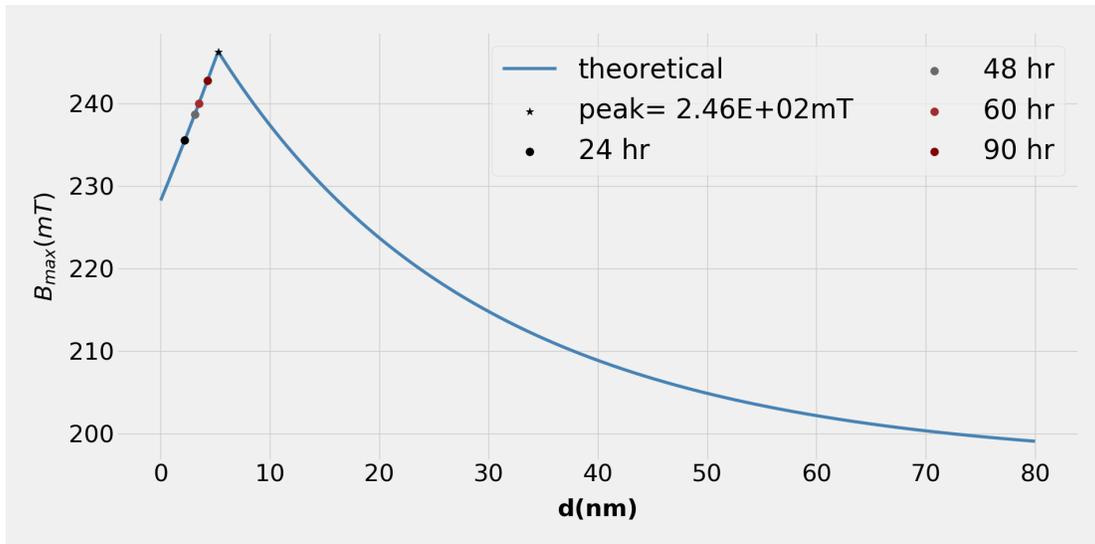
Figure 3.7: Theoretical Simulation of Kubo's Model

The simulation(fig 3.7) shows that the process is still on the increasing slope as far as limitation from dirty layer thickness is concerned.
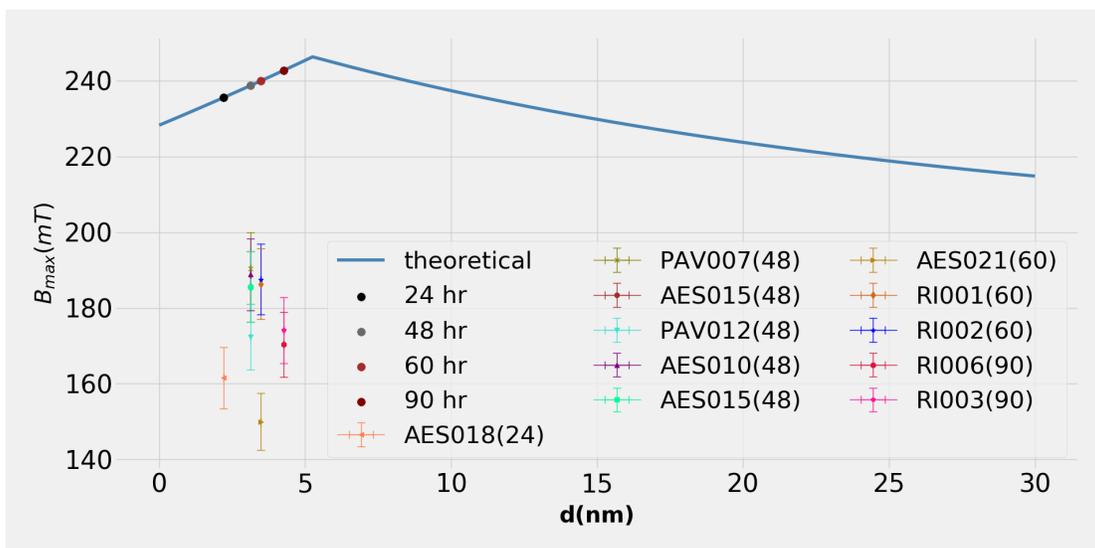
Figure 3.8: Overlaying Experimental data on Kubo's Model

On overlaying the cavities on top of theoretical simulation(fig 3.8) shows that the experimental values don't seem to follow the same trend as is theoretically expected, implying that the cavities are not limited by the dirty layer thickness.

Chapter 4

Conclusion

An efficient software exploiting a BCS fitting routine was developed for extrapolating the average mean free path variation as a function of average depth. This allowed for easy bulk data handling and $\sim 4800\%$ increase in computational speed.

The average mean free path value at the surface and the Nitrogen concentration profile was used to compare the maximum quench field achieved in N-infused cavities with a theoretical model.

Predicted quench field values are higher than what was experimentally measured. Such a discrepancy can be explained by:

- The model was developed in the London limit, which is not the case of clean niobium, so quantitative agreement is not expected

- Presence of local defects that limit the gradient to lower values

- The diffusion constant may have slight changes with time even though theory says otherwise, using only one concentration profile might be a source of errors.

In light of our analysis we conclude that the cavities under study were **not** limited by their dirty layer(global superconductor effects) but most likely by local defects.

4.1   Future Plans

- Acquire more SIMS data to increase confidence in Nitrogen concentration simulation data

- The new code allows for effortless analysis of large amount of data, this can be used to examine more cavities.

- The theoretical model makes assumptions that make true experimental agreement unlikely, a non-analytic reformulation of the theory would result in quantitative confirmation

- Using a diffused boundary simulation instead of a fixed boundary S-S model would give better agreement with experiments

Bibliography

[1] H. Padamsee, "Cavity treatment advances," in <u>RF Superconductivity</u>, pp. 237–261, Wiley-Blackwell.

[2] A. Grassellino, A. Romanenko, Y. Trenikhina, M. Checchin, M. Martinello, O. S. Melnychuk, S. Chandrasekaran, D. A. Sergatskov, S. Posen, A. C. Crawford, S. Aderhold, and D. Bice, "Unprecedented quality factors at accelerating gradients up to 45 MVm 1 in niobium superconducting resonators via low temperature nitrogen infusion," vol. 30, no. 9, p. 094004.

[3] A. Romanenko, A. Grassellino, A. C. Crawford, D. A. Sergatskov, and O. Melnychuk, "Ultra-high quality factors in superconducting niobium cavities in ambient magnetic fields up to 190 mG," vol. 105, no. 23, p. 234103.

[4] A. Grassellino, A. Romanenko, D. Sergatskov, O. Melnychuk, Y. Trenikhina, A. Crawford, A. Rowe, M. Wong, T Khabiboulline, and F. Barkov, "Nitrogen and argon doping of niobium for superconducting radio frequency cavities: a pathway to highly efficient accelerating structures," vol. 26, no. 10, p. 102001.

[5] T. Kubo, "Multilayer coating for higher accelerating fields in superconducting radio-frequency cavities: a review of theoretical aspects," vol. 30, no. 2, p. 023001.

[6] A. Suter, E. Morenzoni, N. Garifianov, R. Khasanov, E. Kirk, H. Luetkens, T. Prokscha, and M. Horisberger, "Observation of nonexponential magnetic penetration profiles in the meissner state: A manifestation of nonlocal effects in superconductors," vol. 72, no. 2, p. 024506.

[7] H. Mehrer, "Continuum theory of diffusion," in <u>Diffusion in Solids</u>, Springer Series in Solid-State Sciences, pp. 27–36, Springer, Berlin, Heidelberg.

[8] M. K. Transtrum, G. Catelani, and J. P. Sethna, "Superheating field of superconductors within ginzburg-landau theory," vol. 83, no. 9, p. 094505.

[9] J. Halbritter, "On the penetration of the magnetic field into a superconductor," vol. 243, no. 3, pp. 201–219.

[10] D. M. Beazley, "Automated scientific software scripting with swig," <u>Future Gener. Comput. Syst.</u>, vol. 19, pp. 599–609, July 2003.

[11] M. Newville, T. Stensitzki, D. B. Allen, and A. Ingargiola, "LMFIT: Non-Linear Least-Square Minimization and Curve-Fitting for Python," Sept. 2014.

Appendices

Appendix A

BCS Processor

Code URL: `https://gitlab.com/ParticularlyPythonicBS/BCS_fitting_Package`

A.1 File Processing

The file processing module is capable of taking in a configuration file and using it to find the relevant data sets and process it for BCS fitting.

The configuration file consists of the name of the file to be processed, the thermometers that are of interest and whether the data needs to be smoothed while interpolating.

The file processor function reads the configuration file and opens each file iteratively. After removing irrelevant data the new data-set consists of the frequency, the quality factor, the chamber pressure, and the relevant thermometers. The frequency is then transformed into the change in frequency by subtracting the initial frequency from the data-set. This data is then cleaned of outliers by constraining the data to removing data over 1.5 times the interquartile range.

The linear regression of the pressure and the change in frequency is used to correct the changes in frequency due to pressure variation.

The change in frequency is then transformed into change in penetration depth by using equation A1.

$$\Delta\lambda = -\frac{g\Delta f}{\mu_0 \pi f_0^2} \tag{A1}$$

The thermometers are then averaged and the duplicate values are removed. The data is then sorted with temperature and this data is interpolated into bins of different temperature scales taking into account the smoothing factor, if specified. Both the processed data-set and the interpolated one are stored separately as final output.

A.2 BCS Fitting

The module for BCS fitting consists of Halbritter C code[9] that is compiled with a python wrapper and python functions for fitting data with the Halbritter function. This dual language approach was chosen since compiled C code is significantly faster which is desirable for computationally intensive parts like solving the BCS model, whereas using python libraries for curve-fitting makes it significantly easier to modify and debug the functionality of the program.

A.2.1 Halbritter code in C

A stripped down version of the Halbritter code capable of using the Temperature and other parameters to give the surface impedance is compiled as a shared library in both Linux and Windows environments.

A.2.2 Python Wrapper

SWIG[10], an interface compiler for connecting C languages to higher level languages is used to seamlessly use the Halbritter functions as a python module

A.2.3 Curve-fitting in python

LMfit[11] ,a python package that allows for easy and modular non linear curve fitting is used to fit data from file processing with the BCS module.
Levenberg-Marquardt minimization algorithm is used for performing the fits.
The BCS fitting generally works the following way:

1. Fitting the data-set covering the whole temperature span for mean free path and gap while using initial guess values for other parameters

2. Fitting mean free path and critical temperature using gap from previous fit

3. Using the critical temperature found to fit a concatenated data-set of all bins to find gap(Physically should be same across all depths/temperatures)

4. The gap and critical temperatures are then used to fit the different binned data-sets to obtain mean free path at each depth

   The fit reports and plots are stored separately for each binned data-set.

A.3 Usage

The file cleaning and BCS fitting are packaged to be easily called from a master program.
   The program can be invoked by typing:

```
python Master.py <parameters>
```

There are 4 legally allowed parameters for Master.

- `python Master.py -h`

Calling Master with the help tag gives the syntax and a brief description of what the different parameters of the function are and how to use them(fig:A.1).
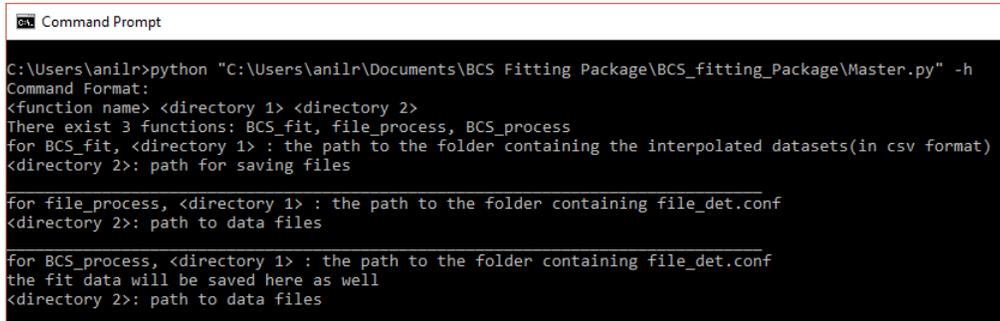
Figure A.1: Calling the console application with help

- `python Master.py BCS_fit <data set directory> <save directory>`

BCS_fit performs BCS fiting on the datasets(.csv) in the data set directory and saves the fit parameters and plots in the save directory

- `python Master.py file_process <file_det.conf directory> <data set directory>`

file_process uses the file_det.conf file and pulls the relevant files from data set directory and saves the interpolated and processed csv files in the file_det.conf directory

- `python Master.py BCS_process <file_det.conf directory> <data set directory>`

BCS_process does the complete process by first calling file_process and then performing BCS fitting on the interpolated files. The fit results are stored along with the file_def.conf

This is the format for file_det.conf:

```
<filename> <thermometers> <smoothing>
% '%' is used in the beginning of a line to skip it
% take care to not skip lines in the file since this breaks the analysis loop
%example
F_Q_te1aes021_20180621_00.txt T1&T2
F_Q_te1RI006_20180523_00.txt T2   760000
% multiple thermometers can be combined with &
% if no smoothing is given, data is simply interpolated
```