ANALYSIS OF SYSTEMATIC AND RANDOM ERROR IN SRF MATERIAL PARAMETER CALCULATIONS*

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Abstract

To understand the relationship between an RF cavity performance and the material on its surface, one must look at various parameters, including energy gap, mean free path, and residual resistance. Though SRIMP fits for seven parameters, three parameters are eliminated using measurement and literature values, and the uncertainty of the fit of the remaining four parameters is further reduced by synthesizing two 3-parameter fits, each from a different data set. To study random error, Monte Carlo simulations were performed of ideal data with added noise; for systematic error, contour plots of normalized residual sum of squares (RSS) of the polymorphic fit on inputted data were generated.

INTRODUCTION

SRF researchers are currently developing new methods, such as nitrogen doping of niobium cavities, and new materials, such as Nb_3Sn, to improve cavity performance. In particular, nitrogen doping is being developed for SLAC's Linac Coherent Light Source II (LCLS II), which will require hundreds of niobium cavities [1]. Nitrogen doping has been found to significantly increase quality factors Q_0, which would significantly reduce associated infrastructure and energy costs for the cryogenic plant [2]; however, the reasons behind this increase in quality factor are not completely understood. In order to gain a deeper understanding of this increase in performance, material parameters and associated uncertainty must be reliably extracted. Similarly, reliable extraction of material parameters of Nb_3Sn can yield insight into this new material. Limitation mechanisms in Nb_3Sn-coated cavities are not yet well understood, so it is imperative to be able to compare critical fields of the material with onset fields for these limitations, but reliable material parameters are needed in order to calculate the critical fields. Furthermore, it is important to characterize Nb_3Sn because its parameters vary widely depending on preparation methods (e.g., temperatures and times); thus, knowledge of its parameters can be used to optimize preparation methods.

For both nitrogen-doped Nb and Nb_3Sn, the parameters of interest are critical temperature, T_c, energy gap, $\frac{\Delta}{k_B T_c}$, intrinsic coherence length, ξ_0, London penetration depth, λ_L, mean free path, ℓ, residual resistance, R_0, and penetration depth at f_0, λ_0. Data on superconducting materials of interest were taken by two different methods: measurement of the quality factor as a function of temperature and measurement of the cavity frequency (f) as a function of temperature. Given either set of data, superconducting parameters can then be obtained by fitting to a model. In this study, J. Halbritter's SRIMP program was used [3], which takes input arrays of temperatures and uses BCS theory equations to compute surface resistance R_s (where $R_s = G/Q_0$, where G is a geometry-dependent constant) and penetration depth λ, which respectively are related to Q_0 and f, for given values of T_c, $\frac{\Delta}{k_B T_c}$, ℓ, λ_L, and ξ_0. Using these 5 parameters, fits can then be made by the addition of constant offsets R_0 and λ_0. However, because T_c can be measured, and ξ_0 and λ_L extracted from the literature, the 7-parameter fit can be reduced to a 4-parameter fit. Furthermore, both sets of data can be fit concurrently to obtain ℓ and $\frac{\Delta}{k_B T_c}$: since λ_0 can be extracted only from the f vs. T data set, and R_0 only from the Q vs. T data set, the sloppiness of the fit can be further reduced by using, rather than one 4-parameter fit based off one data set, two 3-parameter fits—one from each data set—in conjunction with one another. Fitting only f vs. T or Q vs. T yields large uncertainty in material parameters, because either measurement is sensitive to parameters the other is less sensitive to. One of the aims of this paper is to show how the given methods of obtaining parameters such as $\frac{\Delta}{k_B T_c}$ and ℓ minimize their associated uncertainty, and to present a comparison of how the different parameters of interest affect the uncertainty of the fit. Sample fits of Q vs. T and f vs. T data, using the final extracted values for the 7 parameters of interest, are shown in Fig. 1.

METHODS

In order to separately understand the effects of systematic error and random error on the parameters of interest, two methods were used. To look at systematic error from fitting, a range for $\frac{\Delta}{k_B T_C}$ and ℓ were iterated through; the SRIMP-based polymorphic fit was then applied to the data with all values fixed except for constant offsets R_0 or λ_0, depending on which data set was being fitted. The resulting residual sum of squares (RSS) value was saved for each iteration, and a contour plot of RSS, normalized to the minimum, as a function of $\frac{\Delta}{k_B T_c}$ and ℓ was generated. Each call of the polymorphic fitting function used MATLAB's built-in fminsearch function [6] to optimize R_0 or λ_0 after every iteration of the program had run, the resulting array of RSS values was normalized to the global minimum. Because such a contour plot was generated for each of the two data sets, the results from each plot could be synthesized to generate a "combined" contour plot by averaging the normalized RSS values from each data set, and then normalizing these combined RSS values to the minimum.

Monte Carlo simulations were used to analyze and understand random error. SRIMP was used to generate artificial data sets of both types, λ and R_s, from input material param-

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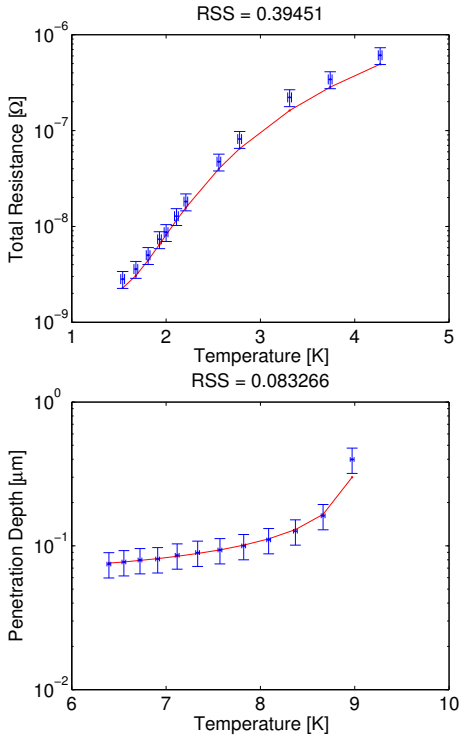

Figure 1: Top: Sample fit of nitrogen-doped Nb using Q vs. T data. Fit parameters: T_c=9.101K; $\frac{\Delta}{k_B T_c}$=1.97; λ_L=38 nm; ξ_0=59.7 nm; ℓ=32 nm; R_0=1.75 nΩ; λ_0=0.16 nm [4]. Bottom: Sample fit of Nb_3Sn using λ vs. T data. Fit parameters: T_c=18 K; $\frac{\Delta}{k_B T_c}$=2.47; λ_L=88.5 nm; ξ_0=11 nm; ℓ=3.25 nm; R_0=9.25 nΩ; λ_0=0.18 nm [5].

eters and temperatures; a predetermined amount of random noise was then added to these data sets after they were generated [7]. The combined fitting program fit both a Q vs. T data set and an f vs. T data set and produced a combined RSS value by normalizing and averaging the RSS value from each. The combined polymorphic fit function was then applied to these artificially generated data sets, and the resulting values for $\frac{\Delta}{k_B T}$, ℓ, etc. were stored for later analysis. For these simulations, a measured value of T_c was used, along with ξ_0 and λ_L values from the literature, while $\frac{\Delta}{k_B T_c}$, RRR, R_0, and λ_0 were allowed to vary. Finally, the fitted value and systematic error were extracted from the contour plots, and random error from the Monte Carlo simulations.

RESULTS

Contour plots of normalized RSS for the polymorphic fit run on each iteration through a fixed range of $\frac{\Delta}{k_B T_C}$ and RRR are presented in Fig. 2 and 3.

The fitted values and systematic error were extracted from the contour plots and the random error was extracted from the Monte Carlo simulations. The systematic error was chosen to include all RSS values within approximately 1 standard deviation (68%) of the minimum RSS. Final fit values for the 3 parameters of interest with their corresponding values for systematic and random error can be found in Tables 1-2.

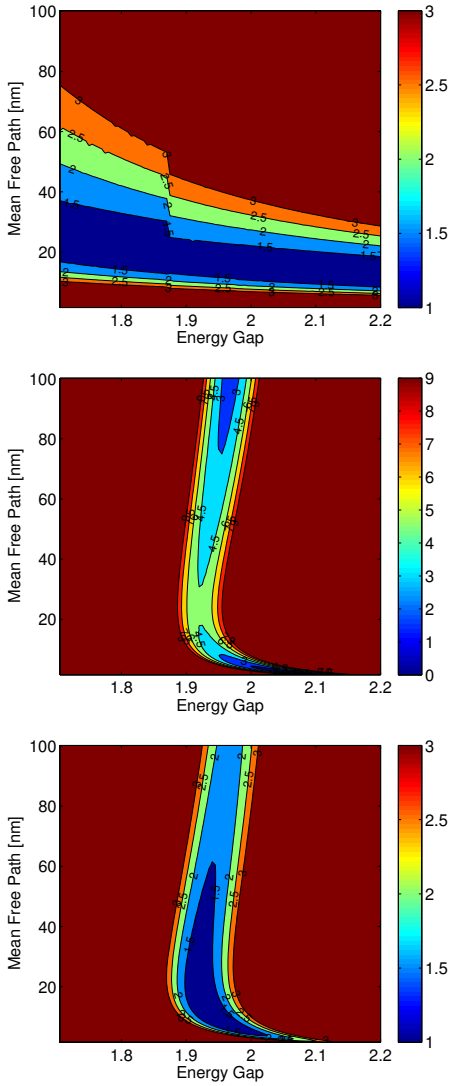

Figure 2: Top: Contour plot of normalized RSS for f vs. T data for nitrogen-doped Nb. Middle: Contour plot of normalized RSS for Q vs. T data for nitrogen-doped Nb. Bottom: Combined contour plot of normalized RSS for nitrogen-doped Nb.

Table 1: Extracted Parameters and Associated Uncertainty for nitrogen-doped Nb.

Parameter	Fit. Value	Sys. Error	Random Error
$\frac{\Delta}{k_B T_c}$	1.97	±0.05	±0.01
ℓ [nm]	32	±30	±2
R_0 [nΩ]	1.75	±0.75	±0.18

DISCUSSION

The trend of λ and R_s with temperature can be approximated by the following equations [8].

$$\lambda = \lambda_L \sqrt{1 + \frac{\xi_0}{\ell}} \frac{1}{\sqrt{1 - (\frac{T}{T_c})^4}} \quad (1)$$

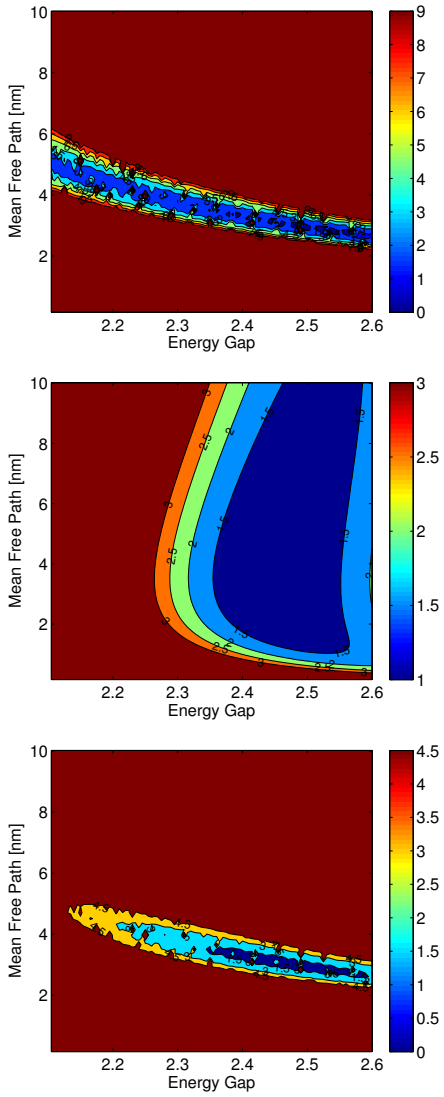

Figure 3: Top: Contour plot of normalized RSS for f vs. T data for Nb_3Sn. Middle: Contour plot of normalized RSS for Q vs. T data for Nb_3Sn. Bottom: Combined contour plot of normalized RSS for Nb_3Sn.

Table 2: Extracted Parameters and Associated Uncertainty for Nb_3Sn.

Parameter	Fit. Value	Sys. Error	Random Error
$\frac{\Delta}{k_B T_c}$	2.47	±0.12	±0.03
ℓ [nm]	3.25	±0.25	±0.12
R_0 [nΩ]	9.25	±1.25	±0.06

$$R_s = \frac{A}{T}\exp\frac{\Delta}{k_B T} + R_0 \tag{2}$$

Since λ is strongly sensitive to ℓ but not as sensitive to $\frac{\Delta}{k_B T_c}$, it is expected that contour plots generated from f vs. T data will not be well-bounded in $\frac{\Delta}{k_B T_c}$, and the range of optimal RSS values will span the horizontal axis. On the other hand, R_s is strongly sensitive to $\frac{\Delta}{k_B T_c}$ but not as sensitive to ℓ, so contour plots from Q vs. T data will be poorly bounded in ℓ, and the range of optimal RSS values will tend to span the vertical axis. Combining the two results into one plot yields results that are more tightly bounded in both $\frac{\Delta}{k_B T_c}$ and ℓ, and thus allows for a reduction of the systematic error associated with both parameters.

CONCLUSION

This project yielded a reliable method of parameter and uncertainty extraction for materials on the surface of superconducting RF cavities. Fitted values and systematic error were taken from contour plots that effectively showed goodness-of-fit as the z-variable and $\frac{\Delta}{k_B T_c}$ and ℓ, two material parameters of interest, as the x- and y-variables. Random error for each parameter was then extracted from a Monte Carlo simulation of artificial data generated from adding noise to ideal values. Furthermore, for all three parameters of interest, systematic error contributes significantly more to overall error than did random error. All in all, this is a very promising method for extracting parameter values for both new materials and new treatments of materials, and an exciting means of gaining new insight that could lead to quality factor improvement in a variety of cavities.

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