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Advanced Topographic Characterization of Variously Prepared Niobium Surfaces and Linkage to RF Losses

Chen Xu
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Advanced Topographic Characterization of Variously Prepared Niobium Surfaces and Linkage to RF Losses

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Doctor of Philosophy

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ABSTRACT

Superconducting radio frequency (SRF) technology is widely adopted in particle accelerators. The shallow penetration (~ 40 nm) of the RF into superconducting niobium lends great importance to SRF cavity interior surface chemistry and topography. These in turn are strongly influenced by the chemical etching "surface clean-up" that follows fabrication.

The principal surface smoothing methods are buffered chemical polish (BCP) and electropolish (EP). The resulting topography is characterized by atomic force microscopy (AFM). The power spectral density (PSD) of AFM data provides a more thorough description of the topography than a single-value roughness measurement. In this work, one dimensional average PSD functions derived from topography of BCP and EP with different controlled starting conditions and durations have been fitted with a combination of power law, K-correlation, and shifted Gaussian models to extract characteristic parameters at different spatial harmonic scales. While the simplest characterizations of these data are not new, the systematic tracking of scale-specific roughness as a function of processing is new and offers feedback for tighter process prescriptions more knowledgably targeted at beneficial niobium topography for SRF applications.

Process development suffers because the cavity interior surface cannot be viewed directly without cutting out pieces, rendering the cavities unavailable for further study. Here we explore replica techniques as an alternative, providing imprints of cavity internal surface that can be readily examined. A second matter is the topography measurement technique used. Atomic force microscopy (AFM) has proven successful, but too time intensive for routine use. We therefore introduce white light interferometry (WLI) approach as an alternative. We examined real surfaces and their replicas, using AFM and WLI. We find that the replica/WLI is promising to provide the large majority of desired information, so that use of the time-intensive AFM approach can be limited to where it is genuinely necessary.

The prevalent idea is that sharp features could lead to magnetic quench or enhance the thermal quench. In this report, a calculation on magnetic field is numerically given on fine structure by finite element and conformal mapping methods. Corresponding RF Ohmic loss will be simulated. A certain thermal tolerant will be calculated. A $Q\sim E$ curve will be predicted from this model.

A perturbation model is utilized to calculate rough surface additional RF loss based on PSD statistical analysis. This model will not consider that superconductor will become normal at field higher than transition field. Therefore, it is only expected to explain mid-field $Q$ performance. One can calculate the RF power dissipation ratio between rough surface and ideal smooth surface within this field range. Additionally, the resistivity of Nb is temperature and magnetic field dependent from classic thermal feedback model theory. Combining with topographic PSD analysis and $R_s$ temperature and field dependency, a middle field $Q$ slope model could be modeled and the contribution from topography can be simulated.
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Chapter 1

Introduction

1.1 Motivation

Superconducting radio frequency technology is widely and increasingly adopted for use in particle accelerators. [1-11] SRF technology applies superconductors, normally niobium or niobium thin film deposited on copper to conventional RF devices for particle accelerators.

As an SRF device, niobium cavity cells have been put into a liquid helium vessel and then surrounded by a vacuum thermal insulating vessel. The RF power has been coupled into the cavity with input RF antenna shown on one side of the cavity. Charged particles entering cavities could be accelerated by the electromagnetic field, usually TM010 mode in side of the cavity. The SRF technology greatly reduces the RF power dissipation on the SRF devices comparing with conventional RF devices. For a continuous electron beam accelerator facility (CEBAF) shape 1.5 GHz cavity or a TeV energy superconducting Linear accelerator shape 1.3Ghz cavity, the RF energy loss of niobium cavity at 2K temperature is 5 orders magnitude lower than that of copper cavity at room temperature. Comparing to normal conducting RF devices, the low RF loss guarantees more of the RF power to be used to accelerate charged particles, ensures the SRF devices possible to work at high duty cycle or even CW mode, and also allows the devices geometry to have larger beam pipe apertures and to minimize deleterious interaction to a particle beam. These properties make SRF technology widely adopted in high average power free electron laser, storage ring and energy recovery linac. Among the various projects that use SRF technology,

1. The Free electron laser Flash program at Deutsches Elekronen Synchrotron in Germany uses 48 nine cell cavities to get 1 GeV electron beam; [1]

2. The X-ray free electron laser program by Desy in Germany uses 800 9 cell TESLA cavities to get 17.5GeV electron beam.[2]

3. The CEBAF at Thomas Jefferson national accelerator facility in US upgrades 80 7cell cavities to the existing 338 5 cell cavities to upgrade the beam energy from 6GeV to 12GeV.[3]

4. The spallation neutron source program in Oak Ridge National lab in US uses 117 6 cell cavities to get 1.3GeV proton beam [4]
5. The Soraq applied research accelerator facility at SOREQ nuclear research center is Israel uses 44 Half wave resonators to get 49MeV proton/deuteron beam [5]

6. Many colliders, storage rings and ERLs that using SRF technology. [6]


8. The Cornell electron storage ring (CESR) [8]


10. The KEKB electron-positron collider at KEK in japan.[10]


12. Accelerator and laser in combined experiments ERL (ALICE-ERL) at Daresbury in UK [12]

13. The BNL-ERL at Brookhaven national lab in US.[13]

The international linear collider is a proposed high energy physics project to collide electron with positrons at 500 GeV but upgradable to 1TeV. This project will use 16000 nine-cell cavities working at 31.5MeV/m gradient to accelerate electron and positron beam to 500GeV separately. The total length of this collider will be up to 31 miles. [13]

With the expansion of SRF technique worldwide, there remains a need for systematic understanding of the fundamental behavior of candidate SRF materials, including niobium treated in different ways and various other bulk/film materials. In order to obtain high Q and large accelerating gradient, a smooth surface should be obtained. Magnetic field can only penetrate superconducting surface within London penetration depth as well as the RF field only penetrates in the length of skin depth. Total effect is that RF magnetic field can penetrate only 40nm in niobium. In this sense, surface resistance will play an important role in RF loss. Exclude surface crystalline and impurity, surface roughness is considered a key part for cavity quality. Researcher took years to achieve smooth surface by various polishing methods. To understand the RF loss, surface impedance is introduced. The real part is surface resistance while the imaginary part is surface reactance. Surface resistance determines the cavity quality factor in typical cavities averaged inherently over significantly all over surface areas. Each surface
process will change the cavity quality in terms of surface resistance. Understanding how surface roughness affects surface resistance will not only improve treatments itself and push the limit of cavities accelerating performance but also enhance the production yield and reduce the total costs. Moreover, niobium, as a type two superconductor, has critical magnetic field $H_{c1}$ around 200mT. This will limit the surface maximum magnetic field thus the accelerating gradient. If locally surface begins to lose superconductivity, the RF loss will increase exponentially. In another sense, the cavities quality factor will drop accordingly. This phenomenon is observed by several laboratories at high field. A tentative model explaining nonlinear Q drop at high field is introduced in this thesis as well as another model explaining linear Q slope at low field.

1.2 Organization of the Dissertation

This dissertation is organized as below:

In Chapter 2, the superconductivity is briefly introduced and niobium superconductivity parameter is given. Different surface polishing on niobium cavities are introduced and compared. Cavity testing methods are briefly discussed.

In Chapter 3, a surface roughness gauge is introduced and adopted to our SRF study.

In Chapter 4, various surface treatments are characterized and compared with PSD technology.

In Chapter 5, Replica and white light interferometry is introduced to this surface study. PSD will be extended into a broader frequency ranges to compare the direct measurement and replica measurement.

In Chapter 6, a model to use PSD to study linear RF loss is given based on electromagnetic wave scattering theory.

In Chapter 7, an advanced nonlinear Q drop model is shown and surface resistance with different treatments are calculated and compared with cavity testing.

1.3 Reference


Chapter 2:
Superconductivity, surface treatments and cavity testing

2.1 Superconductivity and SRF surface resistance

2.1.1 Basics of Superconductivity.

There are two types of superconductors. The fundamental difference is that if the surface energy is positive or negative. This is determined based on the sum of two energies at the near surface region. First energy is the superconducting electrons energy; obviously high electron density will reduce the surface energy at range of coherence length due to its negative potential. The second energy is the magnetic flux, which increase the surface potential at the range of London penetration depths. The combination of two energies will determine if an external flux can enter into the superconductor. If the magnetic flux energy dominates, thus the surface energy is positive and flux is preferably not entering the bulk. This superconductor is named type 1 superconductor. Vise versa, if surface has a negative energy potential then flux can enter surface and it is named type II superconductor. For the type I superconductor, the phenomena that flux are energetically favorable not entering surface is called Meissner effect. Therefore, type i superconductor reveals a total anti-paramagnetic and type II superconductor shows a weak para-magnetics. Ginzburg-Landau parameter is used to describe the ratio between $\xi$ and $\lambda$.

2.1.2 Surface resistance

Skin effect is the tendency of an alternating electric current (AC) to become distributed within a conductor such that the current density is largest near the surface of the conductor, and decreases with greater depths in the conductor. The electric current flows mainly at the "skin" of the conductor, between the outer surface and a level called the skin depth.

The understanding of RF losses in superconducting cavities is very important because cryogenic power will be one of the major limitations for future superconducting particle accelerators. It turns out that RF measurement is very sensitive to the intrinsic properties of a superconductor namely its order parameter. Firstly, from two fluid model, one can deduce from the surface resistance with unit of $\Omega$. Then knowing surface resistance, BCS theory can compute the frequency shift of a cavity as a function of temperature and compare it to experimental measurements.
Finally, this theory points out that impurities and RRR modify surface resistance giving the experimental variation for niobium at 1.5GHz.

A superconducting state has all superconducting electron pairs moving coherently without any resistance. Therefore, this state has low free energy than the normal state electrons. It is required an external energy to excite them into normal states. Such external energy can be thermal electric or magnetic energy. This means if superconductor is subjected to a certain threshold temperature, electric or magnetic field and this energy gap between super/normal electron states will be filled. When superconductor becomes normal state, its resistance abruptly increases 106 times. Even remaining in the superconducting state, the superconductor has non-zero resistance with AC/RF current. This resistance exists only because not all the electrons are superconductor. At high frequency, the normal electrons could not follow the RF field and cause this resistance. This AC resistance is dependent on temperature, energy gap width and frequency. From two fluid model and BCS theory, people have derived equations to calculate this resistance.

Two fluid model presumes that there are two types of electrons in the superconductors: superconductor and normal electrons. When a DC voltage is applied, the superconducting electrons fully short cut the normal conductor. So there is no resistance in DC current transportation. However, if an RF voltage is applied, the voltage changed so fast that neither electrons cannot follow the field instantly due to the inertia; the resistance is present in an RF field. Equation can be adapted as below:

\[
R_S = \frac{A}{T} \sigma_n \omega^2 \lambda^3 e^{-B T_c / T} + R_{\text{residual}} \Delta(T) = \Delta(0) \sqrt{\pi \left( \frac{T}{T_c} \right)^2}
\]

(1)

This equation is independent of purity of material. The penetration depth has a 3-order term, thus has an effective value. The penetration depth is determined by London penetration depth and the material purity \( \lambda = \lambda_L \sqrt{\frac{\xi_0}{\xi}} \). Coherence length \( \delta \) here is introduced generally to estimate how far apart two superconducting electrons are. However, the coherence length is calculated with electron mean free path \( l \) and the pure characteristic coherence length \( \delta_0 \) by \( \xi^{-1} = \xi_0^{-1} + l^{-1} \) and \( \xi_0 = 0.18 \frac{h v_F}{k T_c} \). If the surface is
dirty, then the electron mean free path, which is shorter than pure coherence length is, determine the dirty coherence length. This condition is called 'dirty limit'. The $R_{\text{BCS}}$ is proportional to $I^{0.5}$. On the contrary, on a situation of clean limit, the $R_{\text{BCS}}$ is proportional to electron mean free path.

BCS theory is used to calculate surface resistance at different temperature and frequency at zero electromagnetic field with given parameters such as superconducting energy gap, normal conductivity, penetration depth, and critical temperature. The total surface resistance is calculated by combination with residual resistance. A phenomenological equation can be adapted as below to calculate BCS surface resistance independently from penetration length.

$$R_{s,\text{BCS}} \approx 1.643 \times 10^{-5} \frac{T_c}{T} (f(\text{GHz}))^2 e^{-\frac{1.92 T_c}{T}} \quad (\Omega)$$

With a set of effective surface resistance at different temperature from cavity testing, one can fit the $R$ as a function of $T$ to extract the fitting parameters. Those fitting parameters are used to calculate $T_c$, $\lambda$, $\lambda L$, $I$ and even residual resistance. Previous experience indicates that the surface resistance agrees well with equation above if temperature is less than half of $T_c$. On the contrary, one can extrapolate $\lambda$ at higher temperature by

$$\lambda(T) = \lambda(T_c) \frac{1 - \frac{T}{T_c}}{1 - \frac{T_c}{T_c}}$$

In this way, one can calculate $R_s$ at temperature above half of $T_c$.

The surface resistance vs. temperature data can be fitted according to a quasi-exponential formula that provides a simplified version of the BCS theory, valid for temperatures lower than half of the superconductor's critical temperature or using the full BCS theory with a code originally written by J. Halbritter.[3]

One can see superconductor resistance has frequency quadratic dependency versus normal conducting frequency root dependency.

2.2 Resonator cavity and Surface treatments

2.2.1 Effect of Topography on SRF Performance

SRF performance is usually described by plotting cavity quality factor $Q_0$ and accelerating gradient $E_{\text{acc}}$. In terms of impact, gradient determines
how much accelerator length is needed to achieve the chosen exit beam energy. $Q_0$ is the ratio of the energy stored in the cavity to the power dissipated in its walls, energy that must be removed by the cryosystem. Gradient is the performance challenge for a high energy pulsed accelerator such as the proposed International Linear Collider (ILC). For continuous wave (cw) accelerators of both large and small scale, minimization of dissipated power (maximizing $Q_0$), or more generally, minimizing cryogenic costs, is vital.

Historically, the maximum gradient was often set by turn-on of a field emitter, indicated by a rapid degradation of $Q_0$, with corresponding onset and increase of x-ray emission. On-going progress against field emission relies on reduction or elimination of surface-adhering particles by improved cleanliness and high-pressure rinsing. Quenches without x-ray emission are usually associated with material defects: inclusions, weld beads, etch pits and mechanical damage is severe examples. As with field emitters, reducing the incidence of severe-defect-induced quenches is more a matter of improved manufacturing practice than of scientific discovery. In the push to ever-higher gradients, quenches may occur in the absence of a clearly discernible severe defect. With the application of established processing approaches, cavity wall thermometry during testing can usually associate the quench with a hot-spot near the cavity equator. Such hot spots are viewed as less-severe defects that turn on only at higher surface magnetic fields associated with higher $E_{acc}$. Their specific nature is a matter of current study.

A third class of performance deficit is observed in the push to ever-higher gradients: a decrease in $Q_0$ with increasing gradient – “Q-drop” – with no attendant x-ray emission. Surface topography has long been suspected as a major contributor via magnetic field enhancement (e.g., at grain boundary edges) sufficient to locally exceed the critical field [5]. The resulting normal-conducting volume may be too small to trigger a general quench (in contrast with pits etc.). The cumulative effect of many such small defects turning on with increasing gradient is manifest as reduced $Q_0$ [6]. Recent studies [7] emphasize the importance of intrusions (pits, grain boundary crevices) as well as protrusions. Some of the computational modeling results are surprising. For example a “sharp-edged” (few-micron radius) shallow (depth/diameter < 0.5) disc-shaped pit would have a field enhancement factor between 2 and 3. A viewer would more likely describe surface with such features as moderately rough, rather than pitted. A recent theoretical analysis [8] suggests that thermal feedback may make even apparently-
modest defects more pernicious than thought. A small amount of power deposited at the defect raises the local temperature slightly, increasing the population of normal-conducting electrons. The local surface resistance increases, further increases power deposition until either heat transport out of the absorbing region limits further temperature increase or a quench occurs. Similarly, another model is used to explain SRF cavity quench on the replicated surfaces. [4]

To summarize, smoother is better. “Smother” means eliminating both large, sharp surface features that cause non-field emitter quenches and small features that contribute to Q drop. Further, the smoothest cavity will have the lowest surface area and thus the lowest total surface resistance (for fixed surface character). The desirability of smoothness is not a new insight. What is needed is a more incisive way to measure it and better processes for making it.

2.2.2 Genesis of Nb SRF Cavity Topography

SRF cavities are typically fabricated from 3 mm thick sheet obtained by forging and rolling highly purified ingot stock. Typical grain size is in the 50 micron to 100 micron range, with the (100) and (111) directions normal to the sheet surface. Sheet preparation and cavity fabrication leave several forms of residual strain concentration. These may lead to differences in response to post-fabrication chemical etching, in addition to the effect of attack at grain boundaries and different crystallographic orientation.

Chemical etching (BCP, EP) seeks to remove damaged surface material and to smooth projections. The smoothing obtained by EP of Nb is understood to result from differential attack (leveling) on surface projections owing to a near-surface etchant-depleted layer. The layer thickness is in the range of 8 to 20 microns for typical Nb electropolishing. Surface features much outside this range will not be leveled. At higher temperature (> 30 C), etching appears to grow in importance.

Typical surface topography can be described as 1.) Single-crystal regions several tens of microns in diameter having profuse small steps to accommodate the orientation difference between the crystallographic plane and the macroscopic sheet surface. 2.) Large grain boundary steps due to differential etching of adjacent grains and/or grain boundary attack per se. 3.) Occasional isolated defects, such as pits. 4.) Slow variation at a scale larger than the grain size.
2.2.3 Characterization

The SRF community is developing inspection techniques to detect isolated defects, especially at the cavity equator. Fabrication technology is being improved to reduce the likelihood of their formation.

2.2.4 Standard Procedure

In order to achieve reasonable low surface resistance, one should obtain surface as closed as the ideal condition. This condition includes crystalline, chemical composition and surface topography perspectives. People use quite a few surface treatments such as baking with different temperatures and environments, polishing with different solutions, cleaning with different medium as well as depositing alternative thin film materials. General speaking, baking process promotes the re-crystallization and expelling gas. Cleaning is reducing the adhesive particles and top residual particles. Polishing treatments are smoothing the surface at different special level. After years of experiments, a process procedure is recommended to fabricate state of art ILC 9 cell cavities.

A standard procedure of ILC 9-cell high gradient cavity processing and handling at Jefferson Lab is a summary of the procedure:

- Light BCP etching (10 μm).
- Heavy EP (100-120 μm).
- Post-heavy-EP cleaning.
- Vacuum furnace outgassing (800 °C for 2 hours).
- RF tuning by no-touch bead-pull.
- Post-light-EP cleaning.
- First HPR 3 passes (~6 hours).
- First clean room assembly.
- Final HPR 3 passes (~6 hours).
- Final clean room assembly.
- Leak checking.
• In-situ baking at 120 °C for 48 hours.

2.3 Cavity testing.

As we discuss that the superconducting accelerator has much power loss on the wall at the expense of expensive cryogenic system. The resonators have quality factor $10^9$ above because of the surface resistant is usually under 100 nΩ. However, this quality factor is determined by the averaged surface resistance. There are some explanations that the physical limitation is not reached in reality. Field emission, multipacting and surface roughness are the most popular among those models. Various surface processing and treatments are implemented to achieve ideal surfaces. In order to determine the quality factor of the SRF surfaces, a standing wave testing facility is utilized in Jefferson lab. In cryogenic Dewar system, testing cavities are put vertically, and RF power is fed with RF couplers. A set of powers are measured to determine the energy stored in cavities over energy consumed on the cavity wall. A network analyzer, one RF supplier, two couplers, one circulator and some RF cables are required for cold test. Jlab VTA facility is equipped with a 500W RF supplier which is capable handling 9 cell cavities with reasonable multipacting and dark current. With carefully calibrating supplier and RF cables, one can obtain power forward into cavity, power transmitted out of cavity and power reversed. By determine the coupling parameter $\beta$, one can calculate the $Q_0$. This $Q_0$ is only related with cavity design and cavity surface resistance, and it is independent with how cavities are coupled. The testing diagram is shown below.

To measure the surface resistance of a sample surface, it is essential to put the sample as a part of a resonator. The sample can be fabricated into rods or flat disks inserted to cavity inner surface. One can measure the cavity's global $Q$ so that the surface resistance can be calculated indirectly. In addition, a calorimetric system can be implemented to measure the RF loss directly and equivalently calculate surface resistance. [2] Here we only introduce a universal Cavity vertical cold test which is used in Chapter 7. This cold test concludes that cavity external $Q$ which is related to the cavity coupling and $Q_0$ which is only related to the material surface resistance.

A significant component of JLab's SRF R&D activities is cavity testing and characterization. This is performed in the Vertical Test Area (VTA), a unique facility designed for testing and measurement of SRF cavities in superfluid helium. The VTA consists of 8 dewars, 6 of which are fitted with movable radiation shields, which permits high power testing of cavities without
personnel exposure to ionizing radiation. Cavities can be tested in the VTA at frequencies from 700 MHz to over 7.5 GHz, and at input power levels up to 500W.

\[
\frac{dU}{dt} = -\frac{U}{\tau_L(t)}, \quad \tau_L(t) = \frac{2\pi f_0}{Q_L(t)} \tag{3}
\]

Equation 3 describes that cavity stored energy has a decay time \(\tau_T\) when forward RF is turned off, and this \(\tau_T\) can be calculated from resonate frequency and loaded quality factor.

\[
\beta_i = \frac{1}{2\sqrt{\frac{P_i}{P_r}} - 1}, \quad \beta_i = \frac{1 \pm \sqrt{\frac{P_r}{P_i}}}{1 \mp \sqrt{\frac{P_r}{P_i}}} \tag{4}
\]

where \(P_i\) is the incident power, \(P_r\) is the emitted power, and \(P_r\) is the reflect power in equation 4. These two \(\beta\) factors are calculated from static state and RF turn off state respectively. Then \(\beta = \text{mean}(\beta_e, \beta_i)\). With the measured decay constant and calculated coupling constant, the natural quality factor \(Q_0\) can be calculated from:

\[
Q_0 = 2\pi f_0 \tau_L (1 + \beta). \tag{5}
\]

\(Q_0\) is quality factor that is the ratio of stored RF power and dissipated power in one RF cycle. It is only related to material surface resistance and configuration of field for the excited mode.

We integrate the RF loss of a practical cavity equation below.

\[
P = \frac{1}{2} \times \int_{\text{Cavity}} \int_{\text{Surface}} \left[ R(|H|) \times H(r, z) \right]^2 dS(r, z) \tag{6}
\]

If we simplify that the absolute amplitude of surface \(H\) field is a constant or zero along the axis, we can move the effective surface resistance out of the integrand in equation 13. Thus, the quality factor can be calculated from equation 7.
Take a C100 (CEBAF) cavity as an example, this type of 7-cell cavity is used for Jefferson lab 12Gev upgrade. Its simulated in Superfish is shown in figure below. The surface H field is illustrated in Fig 3 along the axis direction. In Fig.3, blue curve is cavity profile while red curve is surface H field normalized to the peak H field. The H field abruptly changes cavity iris area but the absolute amplitude remains, thus we can use geometry factor in equation below to calculate Q at given H field.

\[
Q_0(H) = \frac{\omega_0 U}{P} = \frac{1}{2} \frac{\omega_0 \mu_0}{R(H)} \cdot \frac{\int H^2 dv}{\int H^2 ds} \equiv \frac{G}{R(H)} \quad (7)
\]

Geometry factor of this cavity is calculated by . The geometry factor is 280 Ω.

The objective of SRF cavity is to push high Q0 at high accelerating field. This is achieved by reducing the surface resistance. Different surface treatments are used to achieve low surface resistance. They are described in details in following chapters.

2.4 Reference:


2. Xiao, B.P., et al., Radio frequency surface impedance characterization system for superconducting samples at 7.5 Gl-lz. Review of Scientific Instruments,

3. J. Halbritter, "FORTRAN Program for the computation of the surface impedance of superconductors", KFK-Extern 3/70-6, Karlsruhe, 1970


Fig 2.1 Vertical Testing Area in Jlab.

Fig 2.2: Surface magnetic field is illustrated on CEBAF 7 cell cavities from Superfish simulation.
Fig. 2.3: Block diagram of a typical cavity testing structure. Courtesy of T. J. Powers, "Theory and Practice of Cavity RF Test Systems", Proceedings of the 12th International Workshop on RF Superconductivity", Ithaca NY, July 2005.
Chapter 3

Enhanced Characterization of Niobium Surface Topography

3.1. Background and Motivation

Particle accelerators continue to grow in importance as tools for scientific research, with applications from the most fundamental physics to user light sources. In many applications, superconducting radiofrequency (SRF) accelerator technology delivers improved performance over traditional technology such that SRF's role continues to expand. The ever-scarce resources for new facilities could go further if their cost could be reduced on a relative basis by increasing SRF performance. The performance of such accelerating structures is usually described by plotting the cavity quality factor Qo versus the accelerating gradient Eacc [1]. In terms of impact, Qo is the ratio of the energy stored in the cavity to the energy dissipated in its walls, energy that must be removed by the cryosystem. Gradient determines how much accelerator length is needed to achieve the chosen exit beam energy. Gradient is the performance challenge for a high energy pulsed accelerator such as the proposed International Linear Collider (ILC). For continuous wave (CW) accelerators of both large and small scale, minimization of dissipated power (maximizing Qo), or more generally, minimizing cryogenic costs, is vital. Two types of performance deficits observed in the push to ever-higher gradients are: 1, a decrease in Qo with increasing gradient – "Q-drop", when a certain gradient is reached; 2, a lower Qo than expected at all gradients.

Surface topography has long been viewed as a major contributor via magnetic field enhancement (e.g., at grain boundary edges) [2]. Even when this enhancement is not sufficient to induce a full quench of the resonance, it may change the local loss. Though the resulting normal-conducting volume may be too small to trigger a general quench, the cumulative effect of many such small defects turning on with increasing gradient would be manifest as reducing Qo [3] at higher gradient. Recent studies [4] emphasize the importance of intrusions (pits, grain boundary crevices) as well as protrusions. Some of the computational modeling results are surprising. For example a “sharp-edged” (few-micron radius) shallow (depth/diameter < 0.5) disc-shaped pit would have a field enhancement factor between 1.5 and 2 [2,5,6]. Chemically-produced etching features on niobium with edge radius of curvature as low as 50 nm have been reported [5]. A recent theoretical analysis [6] suggests that thermal feedback may make even apparently-modest defects more pernicious than once thought. A small amount of power deposited at the defect
raises the local temperature slightly, increasing the population of normalconducting electrons. The local surface resistance increases, which further increases power deposition until either heat transport out of the absorbing region limits further temperature increase or a quench occurs. Efforts to explicitly model the effect of topography continue [7]. Nonetheless, a clear consensus exists in the SRF community that smoother is better and that a more sophisticated analysis is called for.

The topography present on the interior surface of SRF cavities arises from the action of the preparation steps on the typical fine-grained (~50 μm grain size) niobium sheet material from which they are made. As described at length elsewhere [8], the sheet stock is cut, shaped and welded, then polished mechanically and chemically etched. Other forms of mechanical polishing are being replaced by centrifugal barrel polishing, wherein a specially-designed abrasive medium is placed within the cavity and then tumbled to obtain a uniform surface condition. Cavity etching has been accomplished by buffered chemical polish ("BCP"), consisting of flowing a 1:1:2 mixture of hydrofluoric, nitric and phosphoric acids through the cavity at 10°C, removing a few microns per minute up to a total of about 100 μm. Seeking greater final smoothness, BCP is now being replaced by electropolishing (EP) in a typically flowing 1:10 mixture of hydrofluoric and sulfuric acids at 20 – 35 °C, with best results obtained at the lower temperatures [9]. While there are exceptions, gradients in excess of 35 MV/m with quality factor of about 10^{10} are viewed as routinely attainable by EP but not BCP. Fig. 1 shows optical images of typical surfaces as received and after etching.

In these images, it is evident that the surface of the as-received material is significantly transformed by either BCP or EP. BCP shows prominent grain boundaries with smaller hillocks or facets within. EP shows only moderately delineated grain boundaries. Topography at a dimensional scale smaller than several microns cannot be discerned at this magnification.

3.2. Characterization and Methodology

3.2.1 Topography Characterization

Crediting as valid the notion that "smoother is better", there is need for a clear definition of smoothness and its measurement as it relates to SRF performance and cavity processing. Surface topography is routinely measured by stylus profilometry (SP) and atomic force microscopy (AFM). In either case, a probe is moved to a series of locations along a line on the surface and its vertical position is measured. The difference between the vertical position at any specific point and the average vertical position of all points can be computed. Its root mean square (RMS) value, R_q, is one
of the simplest descriptions of roughness [10]. The referenced standard indicates a scan length over which \( R_q \) should be measured. It is not appropriate for the niobium materials, which have an inherent potential non-uniformity at the scale of the grain size, 50 – 100 \( \mu \)m here. Another root mean square (RMS) value \( R_{dq} \) is used to measure slope fluctuation, the \( R_{dq} \) is defined by slope angle of six adjacent points in [11] as:

\[
R_{dq} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \Delta_i^2}
\]

(1)

\[
\Delta_i = \frac{1}{60dx} (y_{i+3} - 9y_{i+2} + 45y_{i+1} - 45y_{i-1} + 9y_{i-2} - y_{i-3})
\]

(2)

where \( y_n \) are the height of adjacent points, \( dx \) is the step length; \( N \) is the total number of points.

Studies of BCP treated niobium reported typical roughness values of 1.6 \( \mu \)m, with a standard deviation of about 0.2 \( \mu \)m [12]. The same researchers reported values for EP of 0.1-0.3 \( \mu \)m, depending on specifics. Further insight can come from viewing the distribution of vertical displacements from the average. Figs. 2 and 3 present the height histogram and the AFM scan profile of typical BCP and EP surfaces. The BCP samples have more height range than do the EP samples.

The value of average roughness can be strongly impacted by the lateral distance over which data are collected. A previously reported comparison of niobium SRF materials treated in different ways found that \( R_q \) values increased more than four-fold as the sampled area increased from 20 \( \times \) 20 \( \mu \)m to 1000 \( \times \) 1000 \( \mu \)m [12]. Use can be made of the variation of \( R_q \) with scan length to acquire lateral information [13]. For the present materials, it may be expected that scan lengths less than the grain size will tend to reflect intra-granular information, while longer will include the grain boundaries as well, as seen below.

A further way to view AFM or stylus profilometer data is to decompose the whole scan into segments of chosen length and then determine \( R_q \) for each segment. The likelihood of including (e.g.) a grain boundary increases with segment length, and the slope in Fig.4 shows this proportionality up to some lateral length. Once the segment length reaches a value where the number of grain boundaries per unit length is substantially constant, the curve flattens considerably. The notable feature in this data is that after electropolishing at - 30\(^\circ\)C, essentially no
dependence on segment length is seen, providing evidence of nearly complete leveling.

Similar to the electropolished surface, the results from BCP in Fig. 5 indicate that there is a saturated $R_q$ at certain scanning length. This distance, larger than which the topography values are substantially constant, may be defined as the correlation length. Visual inspection suggests a value a little less than 80 µm, consistent with the 50 – 100 µm grain size. The correlation length can be more precisely determined by use of an autocorrelation function (ACF) [15]. Defining $h(x)$ as the difference between the height value at $x$ from the average value, ACF can be defined as:

$$ACF(L) = \int_{0}^{L} h(x)h(x+L)dx$$

where $L$ is a fixed distance added to all values of $x$ and $h(x)$ is the profile function. The highest value of $L$ for which the value of the integral is constant is the correlation length. At the correlation length (CL), the value of the ACF falls toward zero. An appropriate scan length for ACF determination 3 – 4 times its expected 75 µm value, here about 200 µm, not the 100 µm scan length limit of our AFM. Calculating the ACF from datasets in Fig. 5 gives a CL value around 30 µm, noticeably too small. Typically, correlation length is proportional to grain size, 20-50 µm in fine-grained Nb. Therefore, measuring it requires at least a 200 µm scan length, preferably 3 to 4 times the correlation length.

Deeper insight into topography can be obtained by considering the variation in vertical position between adjacent measurements, expressed as slope, to capture the notion of sharp features. Histograms are usually used to determine the structure of surface, revealing isolated feature such as holes or bumps. Fig.6 is the slope histogram of scans of Nb surfaces treated by BCP or EP.

The greatly increased frequency in the number of high-slope points for BCP reflects what is qualitatively evident in the optical images earlier. It needs to be understood that the value of slope is affected by the distance between adjacent points. Spacing the points more closely would result in higher slope values for very sharp features, the very ones thought to be most harmful for high-field SRF cavity performance. Further, the sampling issue noted earlier still applies—collecting data from a larger area
increases the likelihood that a point of still higher slope will be detected. Finally, the “fatal flaw” impacting SRF performance is likely to be an extreme point, such as the most prominent sharp projection. From that perspective, the distributions such as Figs. 2 and 6 may be more informative than the various averages. All the statistical methods above are limited by the scan length and characterization resolution, and give no roughness information at different scales.

3.2.2 Power Spectral Density (PSD) Data Analysis

The optics and the microelectronics communities encountered the need to deal more incisively with topography data some years ago [15]. They found it fruitful to make a Fourier transform of the scanning probe topography data to obtain the contribution at different lateral scales: the power spectral density (PSD). Sharper features will have more relative contribution at shorter scales as compared with gentle undulations of the same vertical amplitude, for example.

Power spectral density has been used as a tool to combine measurements from different scales and different instruments [12,15,16]. It represents the spatial-frequency spectrum of surface roughness measured in inverse-length units. The power spectral density function of a surface profile \( h(x,y) \) is defined as [12,15,16].

\[
PSD(f_x, f_y) = \lim_{L \to \infty} \frac{1}{L^2} \left| \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} h(x, y)e^{-2\pi i (f_x x + f_y y)} \, dx \, dy \right|^2
\]  

(4)

where \( f_x \) and \( f_y \) are the rectangular components of surface frequencies. From equation 4, we know that the PSD gives information about the relative contributions of all the possible surface spatial frequencies for an ideal measurement of an infinite surface in the limiting case from 0 frequency (an infinite surface) to an infinite frequency (infinitely small structure) [15]. PSD represents the squared amplitude of surface features plotted against the spatial frequency of those features. PSD and ACF are Fourier transform pairs.

In practice, topographic images of surfaces are recorded in the form of digitized data of surface height, which is finite rather than infinite and sampled rather than continuous. The PSD for digitized data in one dimension used in this study is defined by equation 5 [15].
where $N/2 \leq m \leq (N/2)-1$. Equation 5 gives an expression for the $m$th term in the PSD calculated from a profile of $N$ points; it gives PSD amplitude in units of length cubed. There are discrete values of $f_x = m/L$, where $L$ is the measurement length and $x$ in the function of $h(x)n$ takes on discrete values: $x = (L/N)n$. Also, $\Delta x$ is the spacing between data points in the profile, $h(x)n$ are the height values of the profile data points, and $K(m)$ is a book-keeping factor that equals 1 except that $K(\pm N/2) = 1/2$ at the ends of the power spectrum. More complete mathematical descriptions can be found in references [15,16].

A very important connection between $R_q$ and PSD is that one can calculate the $R_q$ distribution over a specific frequency range. The contribution from that scale is a portion of total roughness composition of the whole scan range. Note that integration of the PSD yields the square of $R_q$ over the range of integration [16].

$$\left(R_q\right)^2 \bigg|_{f_0 \rightarrow f_1} = \int_{f_0}^{f_1} PSD(f) df$$ (6)

Four major limitations are involved in PSD calculations from real data [17]: 1) bandwidth limits, 2) aliasing, 3) trending, and 4) statistical instability [18]. In this study, the bandwidth limits of surface profile measurements are determined by the total trace length, sampling interval and various filtering operations. The surface frequency limits included in this study are [19].

$$f_{\text{min}} = \frac{1}{L},$$

$$f_{\text{max}} = f_{\text{Nyquist}} = \frac{N}{2L}$$ (7)

where $L$ is total trace length sampled at $N$ equally spaced points. In practice, bandwidth limits may be extended by acquiring further scans with greater or lesser distance between data points. The issue of the a possible difference in locations scanned needs to be considered.

Any instrument that acquires topography data convolutes its own signature with the data, the machine transfer function, where "aliasing" is a harmful effect. Antialiasing of stylus profilometry is accomplished by introducing a
low pass filter for surface frequencies greater than the Nyquist frequency [20, 22]:

\[
\tilde{M}(f) = \frac{1}{1 + (fd_0)}
\]  

(8)

The value of \(d_0\) is optimized from tip scanning speed, and defined as the spatial wavelength for 50% amplitude attenuation of this low pass filter. We chose to use \(d_0 = 0.862\ \mu m\) as suggested by reference [20] for a stylus profilometer scan with resolution of about 0.65 \(\mu m\).

In order to explore well the fine scale structure evolution with different treatments and avoid a spurious trend which might be due to the presence of surface components with wavelengths longer than the record length [21], a background must be removed from all data to effectively flatten the mean surface - “detrending.” Experience in the optics and semiconductor communities indicates that a suitable approach is to remove a two dimensional third order polynomial from each record before further analysis [19, 28]. Such an approach is promising for relatively smooth surfaces (EP), but major sharp surface steps (BCP) may need to be individually removed - “destepping”.

Windowing is used to eliminate the discontinuity at the two end points, which may otherwise cause error while calculating the Fourier transform [22]. With a window function, the surface fractal property will be correctly shown. In addition, in order to reduce the statistical instability of real data and minimize the measurement errors, a standard way of stabilizing the PSD function is used: averaging. Fig. 7 below shows PSDs calculated after only averaging data. Fig. 8 shows PSD's calculated after additionally addressing antialiasing, detrending and windowing.

For the data shown in Figs. 7 and 8, power spectra for all traces in the fast scan direction were averaged, and the PSD profiles measured at different locations under the same scan condition were also averaged. A Tukey window transform was applied in Fig. 8 in order to eliminate spurious high-frequency noise and maintain the amplitude of \(Rq\) [23]. As shown in the comparison of Fig. 7 to Fig. 8, the surface fractal property will be correctly shown with use of a window function. In order to reduce the impact of the window function on the averaged PSD, a further polynomial-based deconvolution is conducted in Matlab® code [24].

The impact of proper data treatment on the opportunity to combine different data sets is clearly evident by comparison with previous PSD calculation in Fig. 7 [25]. PSDs in Fig. 8 correct artifacts such as the high frequency leveling and the middle frequency “peak”. Certain characteristic features of
such PSD data from Nb BCP samples are evident: 1) power falls with increasing frequency; 2) a significant data range at high frequencies is a straight line on the log/log plot indicating a power law function; and 3) in the lower frequency data range, the frequency dependence of power departs from linear and approaches a constant value.

To summarize, for stylus profilometry or atomic force microscopy, tip size, spacing of points, number of points, and machine characteristics limit precision and contribute artifacts; obtaining an accurate PSD of a surface requires a series of steps:

1. Data acquisition
2. Antialiasing correction: to reduce contribution from machine transfer function, tip size
3. Detrending correction: to reduce contribution from surface curvature – lack of planarity at large scale
4. Windowing correction: to reduce artifacts on transform due to finite length
5. Averaging: to reduce the statistical instability of real data.

### 3.2.3 Components analysis

Researchers [26,27,28] in the optics and microelectronics communities applying PSD analysis have noticed characteristic patterns associated with frequently occurring topographies. For example, a 90° sharp step gives a PSD having the form \( K/f^2 \), a straight line of slope -2 in log-log coordinates. PSD data may be further analyzed in terms of characteristic patterns. Such structures may frequently be described in terms of three idealized models, fractal structure and two superstructure models.

**Power law structure model [29]**

As is evident in Fig. 8, the high frequency portion of the PSD plot for BCP treated niobium surface appears as a straight line on a log/log plot and so can be fit by a power law expression having the form:

\[
S(f) = \frac{K_n}{f^n}
\]  

(9)

Where \( K_n \) and \( n \) are the fitting parameters. Note \( n \) called fractal dimension, is often between 2 to 3, and larger \( n \) means rougher surface. Power law forms arise from fractal surface topography inter alia, a self-affine topography that is self-similar, having key features repeating at successive
dimensional scales, schematically depicted as a Koch curve shown in Fig. 9:

Characteristic fractal structures are associated with specific values of the fractal dimension D, given by \( D = (7-n)/2 \). Integrating the expression for \( S(f) \) yields the fractal structure \( R_q \) and correlation length \( CL \).

\[
R_q = \left[ \frac{K_n L^{n-1}}{n-1} \right]^{1/2}, \quad CL = \frac{(n-1)^2 L}{2(2n-1)}
\]

Where \( K_n \) is the scaling factor, \( n \) is the fitting order and \( L \) is the scan length. [29, 31] Note, however, that the correlation length obtained from the above equation is necessarily bounded by the scan length.

Superstructure Models

1. “K correlation” or “ABC Model” [32,33,34,35]

Structure present at a larger dimensional scale, such as grain size in the present case, may be superimposed on small-scale structure. Such structure has been described in cluster ion beam polishing and in thin film growth [28]. The PSD of such a model is described by:

\[
S(f) = A/\left(1 + (Bf)^2\right)^{(C+1)/2}
\]

A, B, and C are fitting parameters, with \( C > 1 \). It is possible for a surface to have superstructure at more than one scale, each described by such an expression. For such a model, one obtains \( R_q \) and \( CL \) [26]:

\[
R_q^2 = \frac{2\pi A}{B^2(C-1)}, \quad CL^2 = \frac{(C-1)^2 B^2}{2\pi^2 C}
\]

Note that this calculated \( R_q \) and \( CL \) refer to the K-correlation contribution only.

2. Shifted–Gaussian model [36]

The shifted Gaussian model basically described a surface with isolated island-like structures. Rasigni found this in a PSD with structure that fits a Gaussian distribution but with peak shifted [36]. The model gives clear definitions of size, height and periodicity of particles on an otherwise independently structured surface, which in our case can help calculating local \( R_q \) and \( CL \). It has been demonstrated suitable for describing initial
stage of thin film growth models. A shifted Gaussian component to surface roughness contributes to the PSD as:

\[ S(f) = \pi \sigma^2 r^2 e^{-(f-x)^2 / \tau^2 \pi^2} \]  

(13)

where \( \sigma, \tau, \) and \( x \) denoted the height, size and periodicity of superstructures.

For example, the PSD of a BCP treated-surface might consist of a shifted Gaussian at low frequencies reflecting the grain structure and mostly a straight line at higher frequency reflecting the prominent sharp edges. In contrast, PSD data obtained from electropolished materials typically do not exhibit straight lines on a log/log plot but display two regions of strong curvature, as will be seen later. More generally, the PSD of a niobium surface prepared by various methods can be fruitfully decomposed into contributions from each of these types of models [26,28,37,38].

\[
\text{PSD (total)} = \text{PSD fractal} + \text{PSD } K \text{ correlation} + \text{PSD shift Gaussian}
\]

One may optimally fit the measured PSD curves with such components by using the Levenberg-Marquardt least squares method within the chosen frequency regions. Usually, a certain PSD pattern can dominate within a certain frequency range. Thus, one may fit the PSD in this frequency range with only that dominant model. Accomplishing the fit proceeds with awareness of the characteristic forms arising from the surface processing that has been employed, as indicated above, to make an initial guess. Automatic fitting procedures can then be employed to converge on a best fit. Having these fitting parameters, one can derive the physical parameters: fractal dimension, \( K \) correlation \( R_q \) and correlation length, and particles' size, height and frequency, etc, and learn the surface evolution during process.

3.3 Applications and Results

We illustrate with three sets of materials. 1.) Single crystal Nb materials were obtained by cutting from a large-grained ingot; the surface orientation was determined by electron back-scatter diffraction to be \(<110>\). 2.) Fine-grained Nb was standard RRR sheet material used for cavity production. Both of these type samples were polished to great smoothness (nanopolished) by a proprietary treatment (Wah Chang). While the vendor does not disclose the details of their method, we are able to obtain substantially similar results by careful use of metallographic polishing methods. Samples of each type were subjected to 1:1:2 BCP at 10°C to achieve the material removals indicated later. 3.) Some fine-grained samples were subjected to EP after 100 \( \mu \)m removal by BCP.
100 μm by 100 μm areas on each were examined by AFM. AFM measurements were performed as previously [12] using a commercial AFM (Digital Instruments: Nanoscope IV) in a tapping mode using silicon tips with a diameter of 10 nm. The AFM images were captured as arrays of height values with 512 by 512 points. The Rq and Rdq parameters with and without detrending were calculated and shown in the Table 1. Notice that the Rq value decreases after detrending but Rdq is almost unaffected.

Here, the \( R_q \) and \( R_{dq} \) are RMS of height and slope angle.

### 3.3.1 Single crystals

Since grain boundaries are absent, single crystal samples may correspond to the polishing of grain interiors in fine-grained materials. Four single crystal samples with unknown prior history were characterized before and after 30 μm BCP etch. AFM scans were performed on four different locations on each sample. Representative scans are presented in Fig.10.

Surfaces in Fig.10 give an \( R_q \) change from 11nm to 10nm in Table 1, while Fig.10 illustrates that the surface becomes significantly smoother through BCP etching. Even though this visual impact is significant in the AFM image, \( R_q \) almost remains the same. More insight is required for an incisive analysis.

#### 3.3.1.1 PSD results and analysis

The average 1D PSD derived from the AFM scans Fig.10 are shown in Fig.11 a and b to compare the single crystal sample before and after BCP process. They may be fit by a fractal model + K-correlation model + shifted-Gaussian model. Three components are fitted in Fig 11; fitting parameters are given in Table 2.

Three components are fit in Fig 11, fitting parameters are given in Table 2.

#### 3.3.1.2 Discussion

In Fig. 11, the PSD of the single-crystal sample as-received shows a straight line at middle frequencies from 9.0E-5 to 2.6E-4 nm\(^{-1}\), perhaps due to the previous mechanical polishing history. After BCP etching, the PSD amplitude decreases at low frequency and increases at high frequency. This decrease results in AFM image smoothness, while the increase in high frequency comes from the sub-micron feature growth. It is apparent that \( n \), the fractal dimension, decreases after BCP etching. The PSD amplitude from fractal component also is reduced by BCP.
3.3.2 Initial Genesis of BCP topography

A fine-grained niobium sample received a proprietary polish ("nanopolish") by a commercial vendor. We view this treatment as comparable to careful metallographic polishing. The surface topography of these samples was characterized as received, and after 2 min BCP etch at 18°C. Since we are using 1:1:2 standard BCP solutions, the removal rate is ~3 µm/min, so nominally 6 µm materials was removed.

3.3.2.1 Characterization

Four locations for each state were scanned by AFM. Typical AFM images are presented in Fig. 12.

Fig. 12 clearly shows that the sharp features grow and their sizes vary; \( R_q \) increases from 16 nm to 148 nm on these samples. To learn these features profile, one can chose one representative line sectional profile. Fig. 13 shows two representative line profiles before and after BCP from the fine-grained nanopolished sample as shown in Fig. 12 by black lines. They illustrate that the grain boundaries emerge in sharp relief.

Two cursors are placed at potential grain boundary step. Their heights difference is peak to valley at the step feature. Note that the vertical scales are different. Length and angle measurements at the marked steps are given in Table 3.

From Table 3, one observes that the vertical distance grows from 23 nm to 415 nm, while the horizontal distance remains essential constant, so that, the angle slope of step increases dramatically.

3.3.2.2 PSD results and analysis

The averaged 1D PSD derived from the Fig. 12 AFM scans are shown in Fig. 14 to illustrate the BCP process on nanopolished samples.

Fig. 14 is also regionally fit with different model components and the fitting parameters are given in Table 4.

The PSD of the nanopolished fine-grained sample as-received shows a straight line character at mid frequency and superstructure curvature at low and high frequencies, while the PSD of fine-grained sample after BCP reveals a straight line for the majority frequency range. Presuming that nanopolishing is some variant of chemo-mechanical planarization, this could reflect random roughening at a very low level together with the signature of the abrasive. But BCP produces differential etching and creates facet surface features, which follows power law character as...
reflected by the straight line in PSD. In addition, the amplitude of PSD increases substantially around 1E-4 nm\(^{-1}\), this resulting in the \(R_q\) increasing from 16 nm to 148 nm.

### 3.3.2.3 Discussion

Previously measured [40] removal rates in 1:1:2 fresh BCP solutions indicate 6 \(\mu\)m removal here. In Table 3, the increase of greatest height difference from 23 nm to 415 nm at the grain boundary discontinuity suggests a differential etch rate between exposed grain faces of around 200 nm/min. The lateral length is approximately the observed length of grain boundary incline, so that the slope changes from 0.14\(^\circ\) to 6.7\(^\circ\). Therefore, in lateral frequency range associated with grain boundary feature, a 1-dimension averaged PSD spectrum amplitude increases as an overall effect of each individual line evolution. Since the intra-grain roughness is insensitive to the BCP etching (Table 1), its component in PSD increases little.

The impact of BCP is conditioned by the presence of grain boundaries, a candidate for selective attack (see Fig.12 and Fig.13). The PSD from the nanopolished fine-grained Nb sample shows continuing evolution toward straight line character, reflecting a surface structure dominated by step edges. These grain boundary step edges overwhelm the overall frequency domain. The features of most concern for SRF performance are the pronounced sharp edges at the apparent grain boundaries. On the contrary, in case 3.1, the single crystals (which do not have grain boundaries) do not evolve toward the same PSD character under BCP treatment. This suggests the need for a characterization approach that discerns a small number of isolated features (e.g. histograms) as well as an integrative approach that discerns the net evolution of surface character.

### 3.3.3 Fine-grained Nb sample treated by BCP or EP

Nanopolished samples represent the genesis of topography from near perfect mechanical condition; single crystal samples represent etching the grain interior surface. Here, the final set of samples represents a typical endpoint of polishing of SRF cavities in production.

#### 3.3.3.1 Characterization

The samples were subjected to 100 \(\mu\)m removal by BCP and plus 50 \(\mu\)m removal by EP. EP done here was at 30 \(^\circ\)C without stirring. Samples were scanned by AFM at five locations. Representative AFM images for these conditions are shown in Fig.15.

#### 3.3.3.2 PSD Results and analysis
Representative PSDs for these two fine-grained Nb samples are shown in Fig.16; the corresponding component fit parameters are given in Table 5.

3.3.3.3 Discussion

Analysis of the PSD in terms of contributions shows that BCP-treated surfaces are dominated by the fractal or power law component, associated with the presence of sharp edges, perhaps grain boundaries. The response to EP is more complex. Significant smoothing is evident in the spatial frequency range corresponding to $1 - 10 \mu m$, but not longer. The dominant contributions are K correlation at higher frequencies and shifted Gaussian at lower. Strikingly, a few $\mu m$ removal by one process following the other, results in a change to the PSD signature to that of the last-performed process.

3.4 . Conclusion

The PSD approach affords opportunity to examine the contribution of features at different lateral scales to the observed topography. Obtaining a PSD that accurately represents the surface requires collection, preparation and post-correction of suitable datasets. The PSD can be further analyzed in terms of contributions related to topographic models: fractal/power-law, K correlation and shifted Gaussian. Viewing the effect of BCP and EP, individually and sequentially, in these terms provides useful insights. It is particularly interesting that only a few microns removal by one process or the other causes the signature of sharp edges to come or go. The PSD approach is not, however, sensitive to the presence of a small number of prominent features, which are better revealed by height or slope histograms.

3.5 Reference


FIG. 3.1: Optical images of niobium sheet, a.) as-received, b) after BCP, c.) after EP. The white bar at the lower right of each image corresponds to 200 μm. Optical microscopy courtesy of Thomas Kiederowski, Institute for Laser Technology, Aachen
FIG.3.2: Frequency distribution of height difference from mean after BCP (100 μm removal) or EP (50 μm removal) both at 20 °C. The total scanning point number is 262144. The bin for BCP is 25nm and bin width for EP is 5nm.
FIG. 3.3: Topography images created from AFM data a) after BCP and b) after EP treatment, the same samples as in Fig. 2. The horizontal scales are both 100 µm by 100 µm and the vertical scales are 2500 nm and 50 nm, respectively.

FIG. 3.4: Stylus profilometry measurements of $R_q$ of niobium sheet electropolished in 2N sulfuric acid in methanol at the indicated temperature [14].
Fig. 3.5: $R_q$ as a function of AFM scan length for Nb after 100 $\mu$m removal by BCP, average of three samples.
FIG. 3.6: Slope histogram of the scans in Fig. 2. The total scanning point number is 262144. The bin for BCP is 0.25degree and bin width for EP is 0.05degree.
FIG. 3.7: Power spectral density calculated directly from the raw data for the indicated scans collected from fine-grained niobium sheet subjected to 5 minutes of BCP.
FIG. 3.8: Power spectral densities calculated from the same data as Fig. 7, but with the corrections discussed in the text.

Fig. 3.9: Koch curve illustration of fractal structure [30].
FIG. 3.10: AFM scans of single crystal sample 13 in Table 1 a:) as received b:) after 30 µm removal by BCP. Horizontal scale is 100 µm by 100 µm; vertical scale is 100 nm.
FIG. 3.11: Average one-dimensional PSD of single crystal 13, a.) as-received and b.) after 30 µm removal by BCP. The range of fitting for each component is indicated in solid line.
FIG. 3.12: AFM images of: a.) nanopolished fine-grained sample as received and b.) After BCP with 6 μm removal. Horizontal scale is 100 μm by 100 μm; vertical scales are 500 nm and 1500 nm for a and b respectively.
FIG. 3.13: Surface line profiles of nanopolished fine-grained samples: a.) as-received and b.) after 6 μm removal by BCP.
FIG. 3.14: Averaged 1D PSD for nanopolished fine-grained material: a.) as-received and b.) after 6 µm removal by BCP. The range of fitting for each component is indicated in solid line.
FIG. 3.15: AFM images of fine-grained material after: a) 100 µm removal by BCP or b) 50 µm removal by EP. Horizontal scale is 100 µm by 100 µm for both. Vertical scales are 2500 nm and 1000 nm for a. and b. respectively.
Fig. 3.16: Average 1D PSD from fine-grained ample after removal of: a) 100 μm BCP or b) after 50 μm EP. The range of fitting for each component is indicated in solid line.
Table 3.1: Averaged $R_q$ and $R_{dq}$ parameters with and without third order polynomial detrending with AFM scan range 100 μm by 100 μm (unit: nm).

<table>
<thead>
<tr>
<th>Samples</th>
<th>Single crystal 13</th>
<th>Nano polished 10</th>
<th>&quot;Standard&quot; fine-grained 10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Treatment</td>
<td>As received</td>
<td>After 30 fm BCP</td>
<td>Initial (5-6 fm) BCP</td>
</tr>
<tr>
<td>$R_q$ (nm)</td>
<td>14</td>
<td>13</td>
<td>53</td>
</tr>
<tr>
<td>$R_q$ (nm) detrended</td>
<td>11</td>
<td>10</td>
<td>16</td>
</tr>
<tr>
<td>$R_{dq}$ (°)</td>
<td>0.67</td>
<td>1.1</td>
<td>0.38</td>
</tr>
<tr>
<td>$R_{dq}$ detrended (°)</td>
<td>0.67</td>
<td>1.1</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Table 3.2: Fitting parameters of samples (Unit: nm) for Fig. 11:

<table>
<thead>
<tr>
<th>Model: (nm)</th>
<th>K correlation</th>
<th>Fractal</th>
<th>Shifted Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>As received</td>
<td>1.27E+07</td>
<td>1494</td>
<td>2.71</td>
</tr>
<tr>
<td>After BCP</td>
<td>6.52E+06</td>
<td>1577</td>
<td>1.18</td>
</tr>
<tr>
<td>Frequency Range</td>
<td>2.6E-4–2.6E-3</td>
<td>9.0E-5–2.6E-4</td>
<td>1E-6–9.0E-5</td>
</tr>
</tbody>
</table>

Table 3.3: Lateral lengths and angles between given two cursors shown in Fig. 13.

<table>
<thead>
<tr>
<th>Between two cursors:</th>
<th>Nanopolish by Vendor</th>
<th>2 min BCP (6 μm removal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal distance (μm)</td>
<td>9.2</td>
<td>3.5</td>
</tr>
<tr>
<td>Vertical distance (nm)</td>
<td>23</td>
<td>415</td>
</tr>
<tr>
<td>Angle (degree)</td>
<td>0.14</td>
<td>6.7</td>
</tr>
</tbody>
</table>
### Table 3.4: The fitting parameter of Samples (Unit: nm) for Fig. 14

<table>
<thead>
<tr>
<th>Model (nm)</th>
<th>K correlation</th>
<th>Fractal</th>
<th>Shifted Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>As Received</td>
<td>4.1E+05</td>
<td>1356</td>
<td>1.2</td>
</tr>
<tr>
<td>Frequency Range</td>
<td>4.5E-04~2.5E-03</td>
<td>1.2E-4~4.5E-4</td>
<td>1E-05~1.2E-04</td>
</tr>
<tr>
<td>6 μm BCP</td>
<td>0.16</td>
<td>2.98</td>
<td>27.48</td>
</tr>
<tr>
<td>Frequency Range</td>
<td>1.5E-4~2.5E-03</td>
<td>1E-05~1.5E-04</td>
<td></td>
</tr>
</tbody>
</table>

### Table 3.5: Fitting parameters (Unit: nm) for Fig. 16:

<table>
<thead>
<tr>
<th>Model (nm)</th>
<th>K correlation</th>
<th>Fractal</th>
<th>Shifted Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>100 μm BCP</td>
<td>1.1E-4</td>
<td>3.6</td>
<td>1.1E+012</td>
</tr>
<tr>
<td>Frequency Range</td>
<td>1.5E-04~2.5E-03</td>
<td>1E-05~1.5E-04</td>
<td></td>
</tr>
<tr>
<td>50 μm EP</td>
<td>6.22E+06</td>
<td>1239</td>
<td>1.9</td>
</tr>
<tr>
<td>Frequency Range</td>
<td>2E-04~2.5E-03</td>
<td>1E-03~2E-04</td>
<td>1E-05~1E-04</td>
</tr>
</tbody>
</table>
Chapter 4:

A topographic power spectral density study of the effect of surface treatment processes on niobium for SRF accelerator cavities

4.1. Introduction

Particle accelerators play a steadily increasing role in an expanding range of scientific research. Their greater capabilities and superior cost for performance in many instances result in even more rapid growth for accelerators using superconducting radio frequency (SRF) cavities to power the beam. Niobium is the material most widely used for construction of SRF cavities because it has the highest superconducting transition temperature ($T_c = 9.2$ K) of the pure metals, sufficiently high critical magnetic field ($H_c > 1700$ Oe) for SRF applications, and metallurgical properties adequate for fabrication and service load. The science, technology and history of niobium SRF have recently been reviewed.1

The shallow penetration (~ 40 nm) of the RF into superconducting niobium lends great importance to SRF cavity interior surface chemistry and topography. These in turn are strongly influenced by the chemical etching “surface clean-up” that follows fabrication. The two widely practiced etch technologies are buffered chemical polish (BCP) and electropolish (EP). Typically, BCP solution, the 1:1:1 or 1:1:2 (volume) mixture of HNO$_3$ (69%), HF (49%) and H$_3$PO$_4$ (85%), flows end-to-end through the cavity at approximately 10 °C for a time sufficient to remove the mechanically-damaged and contaminated material, a layer about 100 μm thick.2 Meanwhile, EP uses a 1:10 (volume) mixture of hydrofluoric (49%) and sulfuric acid (96%) at an applied voltage of 14-20 volts. Much work has been done at 20 – 35°C, but lower temperatures appear to yield a smoother surface.3

The Meissner effect excludes the RF magnetic field from the superconducting Nb cavity. The field is parallel to the cavity surface and most intense at the equator. It must deflect to accommodate any topographical features on the surface, raising the local intensity. If the local intensity exceeds the critical field, a local loss of superconductivity results. Absorption there of RF power causes local heating, expanding the affected volume. Repeated many times over the cavity surface, quality factor $Q_0$ is then reduced, more so at higher gradients. The SRF community seeks to move beyond this qualitative description to a quantitative understanding of the effect of topography sufficient to guide cavity processing.
To correlate topography and performance, a means of acquiring and analyzing topography data is needed. Data acquisition so far has been by stylus profilometer (SP) or atomic force microscopy (AFM). The data set is the vertical position of the probe at the sequence of lateral positions comprising the scan. Data analysis may be so simple as the average displacement from the mean vertical position ($R_a$, roughness), which has proven insufficiently incisive for SRF purposes. The next level of analysis is to condition and Fourier transform the scan data to display the contribution at each lateral dimension, the power spectral density (PSD) \(^4\). The approach can be extended by separating the PSD into contributions related to families of surface features, as is done in the optics community\(^5\). These and related analyses probe the average characteristics of the surface. They are relatively insensitive to a small number of singular features, though a single major protrusion or pit may cause poor cavity performance. For these, a kind of approach that views singularities is needed \(^5\).

We report here four sets of experiments relevant to SRF cavity processing to show what can be revealed by the more extensive data processing approaches.

4.2. Experimental methods

4.2.1 Materials

SRF cavities are typically fabricated from fine-grained (“FG”, 20–50 µm), 3 mm thick niobium sheet; its manufacture has been described recently\(^1\). In current practice, after fabrication is complete, the cavity is subjected to BCP etch sufficient to remove mass equal to ~150 µm thickness from the interior surface, annealed at 600–800°C in vacuum to remove hydrogen, subjected to EP sufficient to remove mass equal to 30 µm, and then baked at 125°C in vacuum for 24–48 hours\(^6\). The FG specimens used here were cut from untreated sheet of 10 by 10 mm square.

The possibility that grain boundaries may exert harmful effects, e.g., trapping impurities, has led to interest in fabricating cavities from the largest possible grain size, even single crystals. The vendors have responded by producing Nb ingots that are single crystals or have a large central grain surrounded by smaller grains at the periphery. Slices of suitable thickness are cut by (e.g.) wire saw; the individual grains are clearly identifiable by orientation luster. The single crystal specimens (“SC”) used here were cut by electrical discharge machining (EDM) from within a large single grain and determined by electron backscatter diffraction (EBSD) to have a <110> surface orientation.

Some materials were examined as-cut, having the same surface finish as cavities in production (as-received, “AR”). Others were subjected to careful polishing typical of preparation for metallography (nanopolish, “NP”).
4.2.2. Treatments.

4.2.2.1. Genesis of topography in BCP etching: The effect of grain boundaries

Many researchers, including ourselves\textsuperscript{2}, have shown images of polycrystalline niobium etched by BCP. These surfaces exhibit roughness on a vertical scale on the order of a few microns and a lateral scale comparable to the grain size, leading some to conclude that preferential etching is responsible. We examined four single crystal specimens as-received, the same four after 30 μm removal and the same four after a further 100 μm removal.

4.2.2.2. Genesis of topography in BCP etching: Initial effect of etching

Two nanopolished FG specimens were examined as-received, after BCP for a time expected to remove 3 μm and the same two after a time expected to remove a further 3 μm.

4.2.2.3. Smoothing in EP: Initial smoothing

Four FG specimens subjected to 100 μm BCP were then subjected to EP treatments at 20°C expected to remove 5 μm, 10 μm, or 15 μm, one each. These conditions were chosen to explore the start of EP in the latest current production etch practice.

4.2.2.4. Smoothing in EP: Cumulative heavy etching

Four FG materials, previously subjected to 100 μm BCP, were subjected to EP treatments at 30 °C, removing mass equivalent to 12 μm, 24 μm, 36 μm or 48 μm, spanning the production range. The higher temperature was used here because it is typical of most previous reported work.

4.2.3. Characterization

As previously\textsuperscript{4-5}, the topography was examined by a Digital Instruments Nanoscope IV AFM using tips with diameter <10 nm, eigenfrequency 75 KHz and Young’s modulus 7.5 NanoN/m. A typical AFM dataset consists of 512 scans of 512 data points each. The lateral resolution of the AFM is determined by the distance between sampling points. So for a 100 μm scan of 512 points, the resolution is 100 μm / 512 = 195 nm. Two areas were scanned on all AR materials and at least four on all that were treated. When Stylus Profilometry (SP) was used, the measurements were obtained with a KLA-Tencor P-15 instrument with a 2 μm diameter tip. The samples were scanned
in three different regions each, with scan sizes of 1000 μm × 1000 μm, and the 1000 μm × 1000 μm scan was taken as an array of 251 traces with 2501 points.

4.2.4 Data analysis

An initial way to view the data is in terms of familiar roughness numbers. Because a given sample might have curvature as well as the topographic features of interest, it can be useful to remove a simple polynomial background from the data set before determining the roughness numbers: detrending. Only after background correction is direct comparison of roughness values meaningful. In this paper, profile data were all subjected to third order polynomial detrending. Each of the 512 scans in each dataset was detrended and each transform computed, and all 512 averaged to obtain the one dimensional average PSD, as before 4.7. A Root-Mean-Square (RMS) roughness value ($R_q$) can be calculated as the square root of the integral of the PSD. To better reveal the impact of features of a particular lateral scale, the integral can be taken over the corresponding frequency range and compared to the total. In addition, an RMS slope of the profile or local angle ($r_j$) is also calculated according to ISO 25178 8.

\[
R_q = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \Delta_i^2}
\]

\[
\Delta_i = \frac{1}{60dx} (y_{i+3} - 9y_{i+2} + 45y_{i+1} - 45y_{i-1} + 9y_{i-2} - y_{i-3})
\]

Where $y_n$ are the height of adjacent points, $d_x$ is the step length; $N$ is the total number of points. This RMS slope can indicate the extent of local angle fluctuation. Intuitively, a surface with sharp angles will produce more possibility for hot spots because sharp angle features help enhance the local magnetic field above that at which flux enters the niobium and anomalous dissipation begins. An effective method to quantify them is needed.

Because of its wide data range, the PSD is best viewed as a log/log plot. It has been found useful to further analyze the PSD in terms of three families of contributions 5.9.10. 1: Power law, evident as a straight line on the log/log plot. Stepped or “power” law topography can be responsible. For steps, the power law exponent reflects the internal angle; i.e., 90° step results in power law exponent $n = 2$, and smaller internal angles (sharper steps) give higher values. 2: K (or ABC) correlation. K-correlation treats the surface as a Lorentzian height distribution on an otherwise perfect plane. 3: Shifted Gaussian posits islands of a specific height and diameter. They could be adherent particles or an etching artifact. The visual appearance of the latter two components on a log-log plot is a constant value from low frequency to a turning point followed by a steep decline at higher frequency. It is often called a “shelf".
The fitting of the components to the experimental PSD is carried out by minimization of a merit function that is a measure of the difference between the experimental PSD and the theoretical model. Thus if \( P \) is the set of parameters that characterize the model under consideration, the merit function is defined by equation 3, in which the \( PSD_{measured} \) is calculated from the scan, while the \( PSD_{fitted} \) is the combination of the modeled components.

\[
\text{Merit}(P) = \frac{1}{N} \sum_{i=1}^{N} \left[ \log PSD_{measured}(f_i) - \log PSD_{fitted}(f_i) \right]^2
\]  

in this expression the \( f_i \) are the spatial frequencies at which the measured PSD is evaluated and \( N \) is the number of points at which the PSD is sampled. This merit function is a customized form of the chi-square function, widely used in the fitting of experimental data. The customization consists of subtracting the logarithm of the PSD's instead of the PSD themselves. Doing so is necessary because the values of the PSD function can extend over several orders of magnitude so that a direct comparison would give more weight to the spatial frequencies where the PSD value is higher. This form of merit function has been successfully applied to the fitting of angle resolved scattering measurements. Here, we use the trust-region or Levenberg-Marquardt algorithm in the Matlab® toolbox to obtain global minimization best fit.

4.3. Results

4.3.1 Single crystal niobium with incremental BCP treatment.

4.3.1.1 Experimental data:

The \( R_q \) and \( R_{dq} \) calculated from a set of four single crystal samples are presented in Table 1 to show the reproducibility.

In the Table 1, the most important result is immediately evident. All the roughness values are three orders of magnitude smaller than seen for polycrystalline materials. Little change is evident from the initial removal (30 \( \mu \)m) to even more removal than is typical of production (130 \( \mu \)m total). This suggests that BCP etching establishes a characteristic topography which remains substantially constant as the surface recedes.

Also note that the effect of detrending is significant for roughness, but not for angle, since the angle values arise from the local neighborhood while the
roughness values are relative to the mean surface plane of the whole scan. Selected AFM images are presented in Fig 1.

In Fig.1, Note that the surface becomes effectively smooth after 30 μm BCP treatment, moreover, apparent roughness changes little after additional 100 μm BCP treatment.

4.3.1.2 PSD results and analysis:

Fig. 2 presents a direct view of the PSD results. An average PSD was calculated for each state of each specimen; the associated colors are identified in the figure. This conveys a notion of specimen-to-specimen differences. Also plotted in gray are profiles of each state to indicate the span deviation in the statistical data. Even though $R_q$ from 30 μm and 130 μm BCP are almost the same (Table 1), the PSD’s reveal differences, illustrating the benefit of PSD analysis.

The PSD’s of the as-received materials (Fig.2 (a)) display no systematic similarity. Convergence is becoming evident after the first 30 μm removal, most so for frequencies above $10^{-4}$ nm$^{-1}$ (lateral scale 10 μm and shorter). A further 100 μm removal brings further convergence and decreased contribution at the highest frequency (shortest lateral scale). Evidently there exists a surface topography characteristic of BCP etching which begins to be evident even after only a third as much material removal as typical production etching. Moreover, as noted in Table 1, roughness values for these single crystal samples are on the order of three orders of magnitude less than those of typical polycrystalline materials treated by BCP.

Fig. 3 presents the experimental PSD for these materials together with the calculated fits for each. The dominant character that emerges with increased material removal is K-correlation.

In Fig. 3, the contribution having the highest value in each region is indicated by a solid line and was used for the fitting. Generally, the PSD from as-received PSD and 30 μm BCP treated samples are fitted with combination of K-correlation, power law and shifted Gaussian models, while the 130 μm BCP samples are fitted with multiple shifted Gaussian components at low frequency. Table 2 presents the fitting parameters for each of the four crystals at each of the three treatment stages.

4.3.1.3. Discussion:

An important outcome of the PSD fitting is the behavior of the power law component. The exponent ($n$) varies considerably for as-received material. Note that $n = 2$ for a sharp 90° step. After 30 μm removal, $n$ is well below 2,
and no power law contribution is evident after 130 μm removal. The absence of steps is consistent with the roughness value and the notion that steps are associated with grain boundaries, which are absent in single crystals. The absence of a power law component further indicates that single crystal surfaces, proxies for the grain interiors, have no "power" law component of consequence.

4.3.2. Initial BCP treatment NP FG Polycrystalline Niobium

Two nanopolished fine-grain samples were scanned at multiple locations, and $R_q$ values were calculated and are shown in Table 3. BCP here are conducted with durations different from our previous work.  

4.3.2.1 Experimental data:

Table 3 shows that the $F^*$ and $R_d$ increase from 28 nm to 84 nm to 155 nm and 0.4° to 1.7° to 3.8° respectively. The detrending has little effect. This mainly is because the samples were polished ‘superflat’ by vendor as the initial state. Accordingly, there is no major contour on the background, so that third order detrending had little effect on the $R_q$ values. Selected AFM images are presented in Fig 4.

In Fig.4, one can see step features emerge; note that the vertical scales are different in each figure. Especially significant is the development of sharp steps, even at this early stage of etching. Presumably they are grain boundaries, but specific evidence (e.g., EBSD on each side) is needed. A particularly significant aspect is that there appear to be elevation changes from each grain rather than grooves at grain boundaries. The observed topography is more consistent with differential etching of adjacent grains than with grain boundary attack. More can be learned by viewing AFM traces crossing such steps, represented by the black lines in Fig.4.

In Fig.5, two cursors are placed at potential grain boundary. Note that the full-scale vertical distance is different for each plot. Previous work also showed part of this figure. However, more analysis based on Fast Fourier Transform (FFT) has been conducted to explore the mechanism of feature evolution. Length and angle measurements at the marked grain boundaries are given in Table 4.

4.3.2.2 PSD results and analysis:

Average PSD of each sample at each stage is presented in Fig.6.
By viewing the intermediate transition during 'shelf' structure to power law straight line, one can see the PSD increases in amplitude in mid frequency range, 1 μm~10 μm lateral length. This indicates features within that lateral range increase in height.

In Fig 6, the PSD's of the nanopolished FG samples as-received show a straight line character at mid and high frequencies with curvature at low frequencies: nominally a power law and a shelf. Presuming that nanopolishing is some variant of metallographic polishing, this topography could reflect random roughening at a very low level together with the signature of the polishing process (e.g., wheel vibration). The "power" law dimension n for power law and height value from shift Gaussian model both increase. These facts suggest the features at different wave lengths are all growing. However, the differences in fitting numbers suggest the growth rates vary.

4.3.2.3 Discussion:

The impact of BCP is conditioned by the presence of grain boundaries, where differential etching yields topographic changes (see Fig.5). The PSD shows the continuing evolution toward the power law character, reflecting a "power" law or stepped surface structure. The features of most concern for SRF performance are the pronounced sharp edges at the apparent grain boundaries. The single crystals also evolve under BCP treatment, but do not have grain boundaries or a power law component to the PSD fit. Accordingly, the most reasonable attribution of the power law component here is the steps.

As noted above 1:1:2 fresh BCP solutions remove mass at a rate equivalent to a surface recession velocity of 3 μm/min at 25 °C. Two minutes BCP then results in about 6 μm average thickness removal, implying a nominal height difference no more than several microns. In this two minutes however, the step height difference increases from 22 nm→379 nm→414 nm. A large step develops quickly and maintains prominence with further etching. The limited scan length of AFM (100 μm) vs grain size (50 – 100 μm) impedes obtaining a statistically significant assessment of the distribution of step spacing and height. The application of other approaches is needed.

During sequential BCP, the major change in the PSD happens in the 10^-4 to 10^-3 nm^-1 (1 to 10 μm lateral lengths) frequency region. The corresponding lateral length is approximately the observed length of grain boundary inclines. As shown in the Fig. 5, the grain boundary step height changes from 20 nm to 379 nm to 414 nm, and the angle changes from 0.14 deg to 3.9 deg to 6.7 degree, over a lateral scale of several microns. Therefore, within this lateral frequency range, one-dimension averaged PSD spectrum amplitude increases overall. The single crystal results earlier indicate that intra-grain roughness changes little with BCP polishing; its component in PSD is small. As a whole, after sufficient BCP etching, the PSD of polycrystalline material is dominated
by a power law character, reflecting the large, sharp steps. This indicates that even a light BCP could destroy the smooth surface.

Filter and profile reconstruction with PSD and Fourier Transform (FT):
The PSD pattern changes with BCP at different rate at different frequency. In order to investigate what components are changed by this BCP process, we propose to conduct an inverse windowed FT to reveal feature with different lateral length evolving during this BCP etching.

From Fig.6 one observes that major changes in the PSD fall within the $6 \times 10^{-6}$ to $10^{-3}$ nm$^{-1}$ frequency range. To find its contribution to the change, we can reconstruct the surface by inverse Fourier transform of the PSD over this range. That is, using the PSD, one can reconstruct the surface profile corresponding to the selected frequency range to display the features which fall in corresponding lateral space values.\textsuperscript{11,12} PSD, which is the modulus of the FT, will convolute the real and imaginary parts. In order to invert the FT, the cut-off filter is multiplied directly on the FT components, not the PSD, to retain the imaginary part.

Fig.7 reveals features of the profile originating within a specific lateral spatial range. Figure 7 b represents features with length from 1 µm to 16 µm; Figure 7 c represents features with length falling between 195nm and 1µm. There is a dramatic difference between them because BCP preferentially accentuates grain boundaries. One can see that major $R_q$ contribution comes from the low frequency ($1.0 \times 10^{-4} \sim 1.0 \times 10^{-3}$ nm$^{-1}$), while minor contribution is found at higher frequency ($2.0 \times 10^{-3} \sim 5 \times 10^{-3}$ nm$^{-1}$).

4.3.3 Case 3: Initial EP conversion of BCP

Taking the view that process determines topography, how rapidly does a change of process (BCP to EP) reach steady state? Four fine grained Nb samples were subjected together to 100 µm removal by BCP. One was kept as a BCP record and each of others was electropolished at 20°C to remove 5 µm, 10 µm or 15 µm.

4.3.3.1 Experimental data:
A series of 4 fine-grain samples were BCP and EP polished. Resulting $R_q$ and $R_{dq}$ are presented in Table 6.

In Table 6, roughness and local angle show only modest or no change because of the very short EP duration. However, detrending the data reveals that $R_q$ changes, indicating that the background is not flat. Moreover, the non detrended $R_q$ shows no trends of decrease, but detrended ones do, reinforcing the importance of detrending. Selected AFM images are shown in Fig.8.
The AFM micrographs in Fig. 8 show that the rough surface becomes visually smoother and less sharp, and the edge features become round, though RMS values show little change. Another interesting feature in Fig. 8.b illustrates that, at very early stage of EP, small edge steps emerged, while later EP eliminated these features in Fig. 8.c and d.

4.3.3.2 PSD results and analysis:

In Fig. 9, PSD from AFM are fitted. The AFM frequency range is within $2 \times 10^{-5}$ to $1 \times 10^{-2}$ nm$^{-1}$ in frequency.

In Fig. 9, separate PSD are fitted with a combination of three components and corresponding parameters are given in Table 7.

In Fig. 9, after 5 μm removal by EP, the PSD has significantly transformed from power law structure into a shelf structure. The dramatic change is readily evident in the PSD but not in $R_q$. Net removal of only 5 μm cannot be expected to significantly change the height variation, which underlies the roughness values. However, localized attenuation of sharp projections can have a major impact on the power law contribution. Further, the PSD intensity in the frequency range $4 \times 10^{-4}$ – $4 \times 10^{-3}$ nm$^{-1}$ (few tenths to few micron lateral scale) actually increases as material is removed from these samples by the EP.

4.3.3.3. Full EP conversion of BCP:

As a further comparison, another series of BCP-treated fine grained samples were subjected to EP for times typical of SRF cavity production at (the more typically used) 30°C to remove 12 μm, 24 μm, 36 μm or 48 μm. These latter materials have been described briefly previously.6

Scanned sample $R_q$ and $R_{dq}$ values presented in Table 8 and AFM images are selectively shown in Fig. 11. Note the scanned areas are 100 μm by 100 μm.

With these larger removals, roughness and local angle values fall. Fig. 10 clearly shows that sharp edges and steps are removed even at the earliest stage sampled in this sequence of EP processing. In Fig. 10 c, d and e, the edges and steps are inconsequential, while the same very small features come up and become ubiquitous.

PSDs were calculated from Fig. 10, fitted in Fig. 11, and corresponding fit parameters are given in Table 9.

The fitted Shifted Gaussian model indicates reduced island height; while the macro range size (~ 20 μm) and frequency shift of the islands remain stable. This stability may simply reflect the grain size of the material, and the reducing "island" height is the reduction of height variation across individual grains. The
inclusion of SP data here confidently includes a statistically large number of grains.

4.3.3.4 Discussion

While the total roughness values changed little with initial EP (Table 6), a significant change is seen here with more polishing time (Table 8), consistent with the notion that EP first attacks the sharpest edges and then continues to level projections. Again, most of the impact is in the few to few-tenths micron range. Recent evidence indicates a temperature-dependence in EP mechanisms, favoring polishing over etching at some scales at lower temperature, perhaps a factor in the difference evident between Fig. 9 and Fig. 11. Derived data from Table 9 shows a good trend to smoother surface, although the power law value $n$ appears to increase at the mid frequency range together with decreasing amplitude $K_n$. This increase might be explained by different polishing rates at low and high frequency.

We note some character difference between the sample series 3.3.2 and 3.3.3, although they do not fully overlap. We intend to clarify if this is a consequence of differing process temperature in the near future.

4.4. General Discussion

An observation spanning most of the materials examined is that BCP rapidly promotes the emergence of sharp features when grain boundaries are present and that EP rapidly attenuates them. While this qualitative characterization is not new, the harmonic content analysis is. In Case 1, the rapid effect is evident as change in the power law contribution to the PSD before it appears in the simple roughness values. An intriguing question is: what matters for SRF? Simulation is needed as a first step. A desirable experiment is to examine the performance of a cavity subjected to heavy BCP in that state and again after EP sufficient to remove a few microns. It should be paired with the reverse experiment.

Variability is an issue. Even for single crystals processed together, the PSD’s and the fitting parameters differ by more than a half-order of magnitude. Differences are larger when grain boundaries are present, as may be anticipated. Are the observed differences between samples real or are they within-sample differences? Certainly a factor is that the maximum AFM scan area is 100 x 100 µm, not much different from the nominal grain size for FG materials, so grain boundary or grain orientation differential effects may not be thoroughly sampled within a single scan.. A several-fold increase in the area examined for at least a few samples would be a step toward clarity.

Another feature is the crossover of PSD’s for EP and BCP in the neighborhood of 1 µm$^{-1}$. The meaning is that at micron and smaller length scale, BCP is
smoother and the reverse at longer scale. The EP process is understood to accomplish leveling by depletion of the active fluoride ion species in a layer adjacent to the surface having a thickness of a few tens of microns, depending on specific conditions. 4 At sufficiently small length scale, the difference in concentration of the fluoride ion species will be too small to contribute enhanced leveling. On this very fine scale there may be another process that needs consideration.

Finally there is the behavior of the presumed grain boundaries in BCP. What leads to their prominence and what is the underlying mechanism? Can it be explained as differential etch rate due to variation of chemical potential with exposed face of niobium crystal? Indeed BCP needs to be understood with the same level of detail as is emerging for EP. If the roughening can be controlled, BCP has the appeal of being a much simpler process than EP as current practiced.

4.5. Conclusions

Detailed analysis of the topographic power spectral density of processed niobium surfaces sheds additional light on the mechanisms that yield these surfaces and raises further questions, potentially having practical consequence. Significantly more information is needed, but its acquisition by AFM is a truly daunting task. However, we find that polishing duration and temperature can have predictable effects on the evolution of power law features and superstructures at different scale regions in PSD spectra. This predictability may aid in the development of a more thoroughly optimized production process for SRF cavities yielding the best possible performance for accelerators.

4.6 Reference


5. Chen Xu, Hui Tian, Charles Reece and Michael Kelley. Physical review special topics - accelerators and beams accepted.
6. F. Marhauser, A. Burrill, K. Davis, D. Forehand, C. Grenoble, J. Hogan, R. Overton, A. Reilly,
Fig. 4.1 AFM scans of single crystal 13 (a) NP as-received, (b) After 30 μm BCP, (c) after 100 μm additional BCP. Images are 20 μm per division horizontally by 100 nm per division vertically.
Single Crystal 10 before BCP;
Single Crystal 11 before BCP;
Single Crystal 12 before BCP;
Single Crystal 13 before BCP;

Single Crystal 10 After 30um BCP;
Single Crystal 11 After 30um BCP;
Single Crystal 12 After 30um BCP;
Single Crystal 13 After 30um BCP;

Spatial Frequency (nm⁻¹)

PSD (nm²)

Spatial Frequency (nm⁻¹)
Fig. 4.2: The one dimension average PSD from four single crystal samples. (a) NP as received, (b) 30 µm BCP, and (c) 100 µm additional BCP. The gray lines in each are the highest and lowest PSD for each state to indicate the spread in the total data.
PSD (nm\(^2\))

(a) Single Crystal 11
K correlation
Power Law
Shifted Gaussian 2
Shifted Gaussian 1

(b) Single Crystal 11 after BCP
K correlation
Shifted Gaussian
Fig. 4.3: Selected curve fitting PSD with different models (fitting on average 1D PSD) for Table 1 with different fitting components. a, b, c, d show PSD from samples 10, 11, 12, 13, respectively. From left to right figures show the PSD analysis on the same sample subjected from as received, 30 μm removed and 130 μm total material removal by BCP treatment.
Fig. 4.4: AFM images of nanopolished polycrystalline niobium subjected initial BCP. All 20 μm per horizontal division (a) nanopolished, 500 nm per vertical division, (b) after 3 μm removal, 600 nm per vertical division, (c) after 6 μm removal, 1.5 μm per vertical division. A selected line scan profile is chosen from each image and located in black.
Fig. 4.5: Surface profiles of nanopolished polycrystalline Nb samples (a) as received, (b) after few-μm removal by BCP, and (c) after a few μm additional removal by BCP.
(a1) BCP nanosample 10
- Shifted Gaussian
- K correlation 1
- Power law

Spatial Frequency (nm\(^{-1}\))

(a2) 1min BCP nanosample 10
- Shifted Gaussian
- K correlation
- Power Law

Spatial Frequency (nm\(^{-1}\))
Fig. 4.6: Averaged 1D PSD of nanopolished FG samples shown in Fig. 4.
Fig. 4.7: A series of surface of N=512 points (a), original surface; (b), mid-frequency bandpass range 16 \mu m^{-1}-1 \mu m^{-1}; (c), high pass range 1 \mu m^{-1}-195 nm^{-1}.
Fig. 4.8: AFM images from a FG niobium sample (a) after 100μm BCP surface, then electropolished at 20 °C to remove (b) 5 μm, (c) 10 μm, (d) 15 μm. 10 μm per horizontal division and 5 μm per vertical division.
P S D (nm$^3$)

Spatial Frequency (μm$^{-1}$)

(a) BCP 100μm off FG
EP 5um off FG
EP 10um off FG
EP 15um off FG

(b) BCP 100μm off
- BCP Power law
- BCP shifted Gaussian
(c) +EP 5um off K correlation
+EP 5um off Power law
+EP 5um off Shifted Gaussian

(d) +EP 10um off K correlation
+EP 10um off Power law
+EP 10um off Shifted Gaussian
Fig. 4. 9: PSD direct comparison (a) A set of four PSD, (b) BCP, (c) +5μm EP, (d) +10μm EP, (e) +15μm EP PSD with regional fitting. These different short durations electropolishing are conducted at 20 °C and AFM scanned with size 50 μm x 50 μm.
Fig. 4.10: AFM images from a niobium sample with a), about 100 µm removal by BCP, then incrementally electropolished at 30 °C to remove b), 12 µm, c), 24 µm, d), 36 µm, or e), 48 µm. Horizontal scale is 20 µm per division and vertical scale is 5 µm per division.
Fig. 4.11: PSD after different electropolishing durations with initial state of buffered chemical polishing (a) 100 μm BCP, (b) +12 μm EP, (c) +24 μm EP, (d) +36 μm EP, (e) +48 μm EP PSD with regional fitting. These different short durations electropolishing are conducted at 30 °C and AFM scanned with size 100 μm × 100 μm.
Table 4.1: Summary of the effect of BCP treatment on topography of nanopolished single crystals

<table>
<thead>
<tr>
<th>Sample</th>
<th>SC10</th>
<th>SC11</th>
<th>SC12</th>
<th>SC13</th>
<th>SC10</th>
<th>SC11</th>
<th>SC12</th>
<th>SC13</th>
<th>SC10</th>
<th>SC11</th>
<th>SC12</th>
<th>SC13</th>
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<tbody>
<tr>
<td>$R_q$ (nm)</td>
<td>62.3</td>
<td>18.0</td>
<td>7.43</td>
<td>11.9</td>
<td>5.03</td>
<td>5.44</td>
<td>13.4</td>
<td>10.5</td>
<td>8.26</td>
<td>11.5</td>
<td>7.98</td>
<td>4.38</td>
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<td>$R_q$ (nm) detrended</td>
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<td>8.69</td>
<td>5.98</td>
<td>8.55</td>
<td>4.60</td>
<td>4.54</td>
<td>8.01</td>
<td>4.53</td>
<td>7.70</td>
<td>10.1</td>
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<td>$R_{dq}$ (°)</td>
<td>0.99</td>
<td>0.31</td>
<td>0.93</td>
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<td>0.97</td>
<td>0.61</td>
<td>0.88</td>
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<td>0.44</td>
<td>0.32</td>
<td>0.51</td>
<td>0.50</td>
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<tr>
<td>$R_{dq}$ (°) detrended</td>
<td>0.99</td>
<td>0.30</td>
<td>0.93</td>
<td>0.36</td>
<td>0.97</td>
<td>0.61</td>
<td>0.87</td>
<td>0.55</td>
<td>0.44</td>
<td>0.36</td>
<td>0.51</td>
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Table 4.2: The fitting parameters of Single Crystal Samples (Unit: nm) for Fig 3:

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<tr>
<th>Model</th>
<th>K correlation</th>
<th>Power Law</th>
<th>Shifted Gaussian Model</th>
<th>Shifted Gaussian Model</th>
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<td>Frequency range</td>
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<td>1.0×10^-5-1.0×10^-4</td>
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<td>A B C K_n n Height Size Frequency</td>
<td>A B C K_n n Height Size Frequency</td>
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<tr>
<td>As Received</td>
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<td>10 1.5×10^6 1537 1.1 59.9 1.3 3.5 2.6×10^3 1.3×10^4 6.0 7.8×10^3 4.7×10^5</td>
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<td></td>
<td></td>
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<tr>
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<tr>
<td>Frequency range</td>
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<td>A B C K_n n Height Size Frequency</td>
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<td></td>
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<tr>
<td>30 μm BCP</td>
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<tr>
<td>11 1.8×10^6 1506 1.1 0.3 1.4×10^4 1.6×10^5 1.8×10^5</td>
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<td>Frequency range</td>
<td>7.0×10^-3-5.0×10^-3</td>
<td>n/a</td>
<td>2×10^-4-2.6×10^-4</td>
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<tr>
<td>A B C K_n n Height Size Frequency</td>
<td>A B C K_n n Height Size Frequency</td>
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<td></td>
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<tr>
<td>130 μm BCP</td>
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<tr>
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<tr>
<td>12 3.8×10^6 532 1.1 0.4 4.2×10^3 2.2×10^4 1.7 2.9×10^3 2.9×10^5 0.8 1.5×10^4 3.8×10^5</td>
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<td>13 5.7×10^6 583 1.2 0.9 1.7×10^3 1.2×10^4 0.6 5.6×10^3 6.8×10^5 0.4 1.0×10^4 4.1×10^5</td>
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Table 4.3: Summary of RMS values on the effect of BCP treatment on topography of fine-grained, nanopolished polycrystalline niobium.

<table>
<thead>
<tr>
<th>Initial BCP(nm) Samples</th>
<th>Nanopolished</th>
<th>3 µm removal</th>
<th>6 µm removal</th>
</tr>
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<tbody>
<tr>
<td>NP10</td>
<td>35.5</td>
<td>87.1</td>
<td>154.9</td>
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<tr>
<td>NP13</td>
<td>47.0</td>
<td>71.0</td>
<td>98.2</td>
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Detrended

<table>
<thead>
<tr>
<th>Rq (nm)</th>
<th>27.7</th>
<th>46.8</th>
<th>84.1</th>
<th>70.1</th>
<th>154.9</th>
<th>98.1</th>
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<tr>
<td>R dq (°)</td>
<td>0.4</td>
<td>0.9</td>
<td>1.7</td>
<td>2.2</td>
<td>3.8</td>
<td>2.5</td>
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<tr>
<td>Detrended</td>
<td>0.4</td>
<td>0.9</td>
<td>1.7</td>
<td>2.2</td>
<td>3.8</td>
<td>2.6</td>
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Table 4.4: Lateral lengths and angles between given two cursors shown in Fig 5.

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<th>Between two cursors:</th>
<th>Nanopolished</th>
<th>3 µm removal</th>
<th>6 µm removal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lateral distance (nm)</td>
<td>9.2</td>
<td>6.8</td>
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<tr>
<td>Vertical distance (nm)</td>
<td>22.8</td>
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<td>415.0</td>
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<tr>
<td>Angle (degree)</td>
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<td>3.9</td>
<td>6.7</td>
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</table>
Table 4.5: The fitting parameter of two samples (Unit: nm) for Fig. 6:

<table>
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<th>Model</th>
<th>Sample</th>
<th>K correlation</th>
<th>Power Law</th>
<th>Shifted Gaussian</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>Frequency</td>
<td></td>
<td>$4 \times 10^{-4}$-$5 \times 10^{-3}$</td>
<td>$1 \times 10^{-4}$-$3 \times 10^{-4}$</td>
<td>$1 \times 10^{-5}$-$1 \times 10^{-4}$</td>
</tr>
<tr>
<td>y</td>
<td>As</td>
<td>$4.1 \times 10^5$</td>
<td>1.5</td>
<td>1.</td>
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<tr>
<td>Received</td>
<td>NP10</td>
<td>$1.1 \times 10^7$</td>
<td>9</td>
<td>1</td>
</tr>
<tr>
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<td>$8 \times 10^{-4}$-$5 \times 10^{-3}$</td>
<td>$1 \times 10^{-4}$-$8 \times 10^{-4}$</td>
<td>$1 \times 10^{-5}$-$1 \times 10^{-4}$</td>
</tr>
<tr>
<td>y</td>
<td>6 [m off]</td>
<td>$3.8 \times 10^7$</td>
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<tr>
<td></td>
<td>NP13</td>
<td>$3.8 \times 10^7$</td>
<td>7.4</td>
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<tr>
<td>Frequency</td>
<td></td>
<td>n/a</td>
<td></td>
<td></td>
</tr>
<tr>
<td>y</td>
<td>12 [m off]</td>
<td>$0.1 \times 10^5$</td>
<td>2.</td>
<td>7.4</td>
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<td>8.1</td>
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Table 4.6: Effect of initial EP on fine-grained Nb previously subjected to BCP

<table>
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<tr>
<th>100 µm BCP only</th>
<th>Plus 5 µm EP</th>
<th>Plus 10 µm EP</th>
<th>Plus 15 µm EP</th>
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<tr>
<td>$R_q$ (nm)</td>
<td>224.5</td>
<td>257.1</td>
<td>254.7</td>
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<tr>
<td>$R_g$ (nm)</td>
<td>169.2</td>
<td>163.2</td>
<td>162.3</td>
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<tr>
<td>Detrended $R_q$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$R_q$ (°)</td>
<td>2.9</td>
<td>3.8</td>
<td>4.5</td>
</tr>
<tr>
<td>$R_q$ (°) Detrended</td>
<td>2.7</td>
<td>3.4</td>
<td>4.3</td>
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Table 4.7: The fitting parameter of Samples (Unit: nm) for Fig. 9 (Frequency range applicable):

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<th>Power Law</th>
<th>Shifted Gaussian</th>
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<td>$+5\mu m$ EP</td>
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<td>265.7</td>
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Table 4.8: Effect of full EP conversion on fine-grained Nb previously subjected to 100 $\mu m$ BCP

<table>
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<tr>
<th>Rq (nm)</th>
<th>100 $\mu m$ BCP only</th>
<th>Plus 12 $\mu m$ EP</th>
<th>Plus 24 $\mu m$ EP</th>
<th>Plus 36 $\mu m$ EP</th>
<th>Plus 48 $\mu m$ EP</th>
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<td>206.3</td>
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Detrended
Table 4.9: Fitting parameter of Samples (Unit: nm) for Fig. 11 (Frequency range applicable):

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<td>$8 \times 10^{-5}$</td>
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</tr>
<tr>
<td>12 µm</td>
<td>$8.9 \times 10^{-1}$</td>
<td>6.3</td>
<td>13.1</td>
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<td>Frequency</td>
<td>$1 \times 10^{-6}$-$2 \times 10^{-5}$</td>
<td>$2 \times 10^{-5}$</td>
<td>$2 \times 10^{-4}$</td>
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<td>36 µm</td>
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<td>4.3</td>
<td>5.3</td>
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<td>$3 \times 10^{-5}$</td>
<td>$4 \times 10^{-4}$</td>
</tr>
<tr>
<td>48 µm</td>
<td>$5.0 \times 10^{-13}$</td>
<td>5.1</td>
<td>2.6</td>
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Chapter 5:

Characterization of Nb SRF cavity materials by White light interferometry and replica techniques

5.1. Introduction

Superconducting radio frequency (SRF) cavities are continually being improved for present and future accelerator projects. Moreover, improvements can be applied to existing machines as cryomodules are cycled out for refurbishment, offering opportunity to reduce present power costs. Energy consumption is characterized by the cavity quality factor $Q_0$, the ratio of energy stored in the cavity to energy lost (which must be removed by the cryosystem). $Q_0$ is understood to be adversely impacted by surface roughness. 1,2,3 The most pernicious roughness is topographic features having sharp edges as well as large amplitude. A proposed mechanism by which these features exert harm is that they increase the local magnetic field, causing local quenches that absorb power and expand. To avoid this and kindred performance impairment, the interior surface topography would desirably be as smooth as possible by careful monitoring through each stage of production. 4, 5 Monitoring implies interior surface access. Replication offers a step in that direction, transferring the topography of interior surface to a flexible, highly accurate and stable polymer material. This 3D copy of the surface allows microscopic examination and precise surface measurements by established techniques.

However interior access is obtained, topography must be measured. Stylus profilometry is successful down to a few-micron lateral dimensional scale. 5 Atomic force microscopy (AFM) offers higher lateral resolution, down to several nanometers, but takes long acquisition time and covers very limited scanned areas. A new method is needed to acquire far more data so that a systematic picture can emerge.

However obtained, topographic data are frequently analyzed in terms of average roughness amplitudes ($R_q$, $R_a$). Far more detail is needed for SRF purposes. Important added insight comes from viewing the Fourier transform of the data, for typical structures have characteristic spectral signatures,7.

5.1.1 Replica technique

The making of replicas is a way to render accessible for examination surfaces which are otherwise not so 8,9,10,11. Apparently the first reported use was in 1958 for mechanical wear studies 12. Examples now include...
weld joint surfaces at nuclear power plants, corrosion and cracking of gas or liquid pipelines and even biological samples. It has also found application under extreme conditions, e.g., under water or vacuum. Typical microstructures investigated range from a few microns to macroscopic features. The SRF cavity application seeks to push lateral resolution to sub-micron. Replication can be accomplished in either one or two stages depending on the nature of the further characterization. The original single stage process consists of applying cellulose acetate tape softened with acetone. The tape hardens with solvent evaporation and is removed for examination. The hardened tape may not be flat and its transparency can complicate examination by optical microscopy. A careful study found that the lateral resolution limit for cellulose acetate replicas is about 0.25 μm. Further, the replica shrinks by about 1/3 in the vertical direction.

New materials seek better resolution by using proprietary two-component polymer mixtures that do not cure by solvent loss and hence have far less tendency to shrink. However, they do not attain hardness sufficient for the mechanical stresses of stylus profilometry. Accordingly, the first stage replica is used as a mold for a second polymer stage having the desired properties. Since the ultimate lateral resolution may thereby be reduced, the most appealing prospect is examination of the first-stage fresh replica by non-contact characterization methods.

For SRF use purposes, a replica is required to achieve at least micron lateral spatial resolution, but not leave contamination on the cavity surface. The potential contamination, if any, should be RF lossless or removed by high pressure water rinse (HPR). Replica techniques have been used to examine cavity interior surface defects, but evidently not to capture topographic data.

5.1.2 White light interferometry

White light interferometry (WLI) is a non-contact characterization method and thus favorable for the single stage replica technique. WLI has an extensive application history in optics, aerospace, semiconductors and more. The image of a region on the surface is projected by the viewing microscope onto the pixel array of the camera. The lateral spatial resolution is controlled by the relationship between the camera pixel size and the magnification of the viewing microscope, but has an ultimate limit on the order of the wavelength of light, somewhat less than a micron. In practical terms, field of view (FOV) size (how much area is sampled) is traded off against lateral resolution. The importance of understanding the desired information is evident, so that the best parameter choices can be made. WLI is capable of measuring very rough surfaces. Its useful vertical (z) range is...
Some investigators have successfully combined AFM and WLI to span a wider range than either alone. White light Interferometry is conceptually straightforward. The signal intensity in interferometry using a single wavelength goes from a maximum to a minimum to a maximum every time the path length difference (due to surface elevation difference) between the beam from the sample and a reference beam equals a wavelength of the light employed. The same would be the case for any integral number of wavelengths, introducing an ambiguity into the measurement of the difference of surface elevation between different points. This does not occur for white light with its mixture of wavelengths.

In Vertical Scanning Interferometry (VSI) mode the sample moves vertically while each camera pixel records the intensity of the interferometer signal from a specific point on the sample surface. The intensity varies according to the relative elevation of each surface point. The intensity data as a function of the optical path difference (OPD) are digitally recorded as a series of matrices at each moving step. By examining each element in these matrices, the interferometry fringes signal would be like amplitude modulated (AM) communication signals. If the surface elevation varies by less than a wavelength of light or so, phase scanning interferometry (PSI) mode can be used instead.

Averaged PSD are calculated from AFM line raster scans with proper detrending and windowing. Because data acquired from AFM has equal length vertically and horizontally, there is no difference in frequency covered by PSD. However, it is preferred to calculate PSD along with raster to avoid displacement between each line. Rectangle images are obtained from a snap shot WLI, PSD can be calculated from either direction, though PSD from longer side is preferred because it covers longer frequency range. Note images from WLI are not only subjected detrending and windowing, and an image correction may be needed.

5.2. Experimental methods

To gain insight into what may be learned by the replica/WLI approach in contrast with direct AFM, we examined a number of cm-square coupons by both approaches.

5.2.1 Samples

Pitting in Buffered Chemical Polishing (BCP): heavy etching
Large grain niobium samples were cut from sheets which had been cut by wire EDM from ingot material. Without any further annealing or rolling, the
samples were subjected to BCP sufficient to remove 120-150 μm, as described previously 35.

Initial Smoothening in Electropolishing (EP)

Four fine grain Nb specimens were BCP etched 100 μm and further subjected to incremental EP treatments at 20°C, sufficient to remove in total 5 μm, 10 μm, and 15 μm. These materials were described previously. 36 The polishing conditions were typical of those used in the final stage EP in current cavity production.

5.2.2 Replica Materials:

The replica material used here was ‘Repliset’ from Struers (Denmark), comprising a resin and a hardener mixed at the point of application by device provided by the manufacturer. The mixture is opaque and has fair mobility, with a curing time of four minutes at room temperature. Struers claims <0.1 μm lateral resolution, with negligible shrinkage over time. 18

5.2.3 Topography measurement:

In order to maximize lateral resolution, these replicas (negative mold) were examined directly without making a second step positive casting. Because the replica surface is relatively soft, its characterization requires low contact force. We used a Digital Instruments Nanoscope IV AFM with tips having a 75 kHz resonant frequency and force constant of 3 nN/m. For the niobium metal surfaces we used tips with a 300 kHz resonant frequency and force constant of 7.5 nN/m. Inspection of the replicas by SEM after examination showed negligible damage. The pitted surface and its replica were scanned as 12×12 μm areas with 23 nm lateral resolution (scan length divided by number of points). The series of EP samples and their replicas were scanned as 50×50 μm areas (100 nm resolution) at four different locations on each sample.

The WLI data were obtained using a Contour GT-K1/X8 3D white light interferometer from Bruker Nano Inc. operated in phase shifting interferometry (PSI) mode, because our surface is quite smooth compared with its Z range capability. In PSI mode, lateral resolution is determined by the objective lens magnification, camera zoom and pixel resolution. Here a 5 X objective lens magnifications and 1.0X camera magnification were combined to yield a 5X “low magnification” WLI image. A 50 X objective lens magnification and a 0.55X camera magnification were combined to yield a 27.5 X “high magnification” image. Respectively, the resulting lateral resolutions are 1.94 μm and 0.36 μm, with a field of view of up to 1.24mm x 0.933mm and 0.231mm x 0.173mm. 30 The vertical resolution is less than 0.1 nm. Data were collected at five randomly chosen locations. The post-process software Vision 64, transfers from the raw phase/intensity data to S.
I unit and fills any missing data due to, e.g., lack of reflection. Such conversion already includes high order polynomial detrending and optical transfer function correction. The output data format is matrix with 640 x 480 elements.

It should be noted that AFM obtains two-dimensional information by assembling successive parallel scans, while WLI collects fields-of-view and is thus inherently two dimensional. Power spectral distributions (PSD) were calculated from WLI and AFM scan data as in our previous reports.\(^{37}\)

5.3. Results

5.3.1 Resolution determination.

Fig. 1 presents optical images of the real sample and its replica. A grain boundary traverses the center of each image; pits appear profusely to its right side.\(^{35}\)

Simply viewing corresponding real/replica images is useful, but a more quantitative approach is needed. Fig. 2 presents a cross-section of a selected pit and its replica, indicated as the black lines on the AFM images. The horizontal dimensions are 10.49 and 11.52 microns; the vertical dimensions are 1.56 and 1.55 microns and angles are 23.58 and 20.71 °. Features smaller than 500 nm are not well reproduced. A plausible reason is that the tip and replica interaction is too strong, blurring the replica image, even though the Young’s modulus is small and AFM operates in tapping mode.

Such one dimensional and visual comparison is not sufficiently quantitative. The line profile selection always incorporates human judgment as to the precise location. Further, no comparison index is obtained to quantify the replication similarity. In order to obtain a similarity index from actual and replica samples, one needs to properly align the scanned profiles and calculate Local Cross Correlation Function (LCCF) on the targeted features. After the two patterns from real and replicated surface are aligned and scaled, the Local Cross Correlation Function is calculated as\(^{38}\)

\[
c(P, T) = \frac{\text{cov}(T, P)}{\sigma(T)\sigma(P)} = \frac{1}{NT} \sum_{x,y} [P(x, y) - \mu(P)] \cdot [T(x, y) - \mu(T)]
\]

Here, \(\text{cov}(T,P)\) is covariance function and \(c(P,T)\) is the normalized LCCF coefficient. The function \(P\) and \(T\) are topographic height maps from direct and replica measurements, where the \(\mu(P)\) and \(\mu(T)\) are respective mean values and \(\sigma(P)\) and \(\sigma(T)\) are the respective standard deviations of sub-
domains. NT is the number of pixels of both images. When the coefficient equals 1, the replica is a perfect match to the real object.

N. P. Pitsianis in Duke University calculates integration of LCCF and obtains similarity index in Matlab-base software. Red circled pits from Fig. 3 above have normalized LCCF coefficient of 91.75%.

5.3.2. Incremental EP samples

5.3.2.1. Optical microscopy

The prior BCP treatment left a significantly rough surface having large fluctuations in addition to local roughness. The fluctuations contribute the majority of RMS height variation and rough appearance, with little sharp curvature on top. Fig. 4 compares optical images of the BCP treated initial state for the real coupon and its replica. Comparison images of the subsequent increasing degrees of electro polishing appear in the supplemental material.

5.3.2.2. PSD of data from real coupons and replicas

The topography of real coupons in each of the four conditions was characterized by AFM as 50 μm × 50 μm areas. A set of replicas of these materials was similarly examined, save that the scanned areas were 60 x 60 μm. The AFM images from both appear in the supplemental data and generally show increasing smoothness. The data obtained are analyzed in terms of power spectral distribution (PSD) in the same way as previously.

Replica AFM pictures of four are shown below. Different from the previous AFM, the resolution is 117nm with scan area 60 μm×60μm. It covers more frequency range more than previous PSD.

In Figure 6, the noticeable difference between the real and replica PSD's occurs at higher frequencies, where the replicas appear less sensitive to the high frequency components. The highest frequency components arise from sharp edges, which would be the features most vulnerable to deformation by the AFM tip.

5.3.3. WLI examination of real coupons and replicas

The same samples used for AFM characterization as described above were examined by WLI using the parameters in Table 1.
Images obtained from the real coupons and replicas before EP (BCP only) appear in Fig.8. Both sets of WLI images for the sequential EP states appear in the supplemental material. The notable feature in the WLI images here is the large plateaus. Their dimensional scale is too large for the available AFM scan length.

The PSD's calculated from the high magnification WLI data from the real coupon appear in Fig. 7. They are averaged from four different locations on each sample, and these locations are independent of previous AFM. Note that the PSD extends over a far wider frequency range than for the AFM data. The straight line seen in the AFM data from BCP-only is evident in the high frequency range data here. Fig. 9 presents the equivalent data from the replicas.

The PSD's from the real and replica materials are much more the same for topography data collected by WLI than by AFM. This is expected since there is no tip contact to cause distortion in WLI.

5.4. Conclusion:

We find that, when examined by AFM, replicas yield topography information comparable to corresponding real surfaces down to the desired sub-micron lateral resolution, subject apparent distortion by the tip. It is reasonable to expect that further effort to reduce tip/surface interaction and to increase replica hardness will help mitigate this problem. However the problem of time demand will remain no matter what progress is made toward improved fidelity. We find that, when examined by WLI, replicas yield topography information substantially equivalent to that obtained from real surfaces. The area examined is increased and the required time is decreased by orders of magnitude. More remains to fully understand the WLI "view" of the surface topography and how it can best be practiced. Even so, its potential is clear.

5.5 Reference:

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   025302
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Fig 5.1: Stitched optical images of large grain Nb sample (left) and its replica. The major vertical feature is a grain boundary. Red circles indicate identical points chosen for AFM examination (see supplemental material).

Fig. 5.2: Line profile comparison from AFM to determine the lateral resolution of this replica material. A sectional profile with measurements are in red and green between cursors with the same color code.
Fig. 5.3: The cross-autocorrelation comparison and the similarity index in bird's view. The cross correlation function is calculated from two 3D topographic profiles with proper alignment.

Fig. 5.4: Optical images of early incremental EP stages of fine grain Nb and their corresponding replica. (a) initial BCP surface, (b) +5µm EP off, (c) +10µm EP off, (d) +15µm EP off are shown in the supplementary materials. Upper image is direct surface and lower image is the replica. The length legend bar are the same and shown in the Figure 4 a.
Fig. 5.5: AFM images from a FG niobium sample a) after 100 µm BCP surface, then electropolished at 20 °C to remove b) 5 µm, c) 10 µm, d) 15 µm. 10 µm per horizontal division and 5 µm per vertical division.
Fig 5.6: AFM images from a Replica FG niobium sample a) after 100μm BCP surface, then electropolished at 20 °C to remove b) 5 μm, c) 10 μm, d) 15 μm. 20 μm per horizontal division and 5 μm per vertical division.
Fig. 5.7: PSD after different short electropolishing durations are described above.
As reported previously, the straight line (power law) in Figure 5 is characteristic of BCP with its sharp edged features. Even the least EP significantly rounds them resulting in the character seen here; for a detailed discussion see previous report.38
Fig. 5.8: PSD of replica from incremental EP samples after different short electropolishing durations with initial state of buffered chemical polishing (AFM scan size 60 μm × 60 μm)
Fig. 5.9: PSD after different short Electropolishing durations with initial state of Buffered Chemical polishing (WLI scan size 1.24mm × 0.93 mm+0.235 mm × 0.173 mm) at 20 °C. The low magnification WLI PSD has high amplitude at $3 \times 10^{-5}$ to $2 \times 10^{-4}$. This might be because the noise of low magnification objective lens.
Fig. 5.10: 27.5x WLI images from a Replica FG Niobium sample a) after 100µm BCP surface, then electropolishing at 20 °C to remove, (b) 5 µm, (c) 10 µm, (d) 15 µm EP process. (Height scales are shown in the color bar.)
Fig. 5.11: PSD after different short Electropolishing durations with initial state of Buffered Chemical polishing.
Table 5.1: parameters for white light interferometry.

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<th>WLI</th>
<th>(a) Direct low Magnification</th>
<th>(b) Direct High Magnification</th>
<th>(c) Replica Low Magnification</th>
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</tr>
<tr>
<td></td>
<td>8.1×10⁻⁷ nm⁻¹</td>
<td>4.2×10⁶ nm⁻¹</td>
<td>8.1×10⁻⁷ nm⁻¹</td>
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<td>0.49 μm</td>
<td>1.94 μm</td>
<td>0.49 μm</td>
</tr>
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</table>
Chapter 6:

Mechanism of Contribution to Niobium SRF cavities linear RF loss due to topographic surface structures

6.1. Introduction

RF loss induced by roughness is considered in many RF components, such as micro strip transmission line, wave guide and RF resonator. It can be understood that the RF electromagnetic field penetrates the surface, and the induced current will pass and cause RF loss. [1] However, in a RF wave view, the incident wave is reflected, scattered and absorbed by the rough surface. Inside of a resonator, the reflected, scattered wave contributes to standing wave field, while the absorbed RF wave is attributed to the RF surface loss. These two perspectives may both be used to describe the same RF loss.

In a resonator, only several specific RF standing wave modes can exist to meet the boundary conditions, which are determined by the resonator geometry. The total electromagnetic field at each point is a combination of EM components of a series of plane waves. Within the resonator, E and M are separated in space and interchange their energy over a distance. Thus the peaks of E and M fields are always not in the same location. TE, TM, TEM are used to describe the EM field direction relative to the beam axis. Waves are incident to the resonator surface from all directions. Therefore, the RF loss calculation method requires direction independence, and covers all frequencies or wavelengths of incident waves.

6.2 Methodology

Rough surfaces will cause more RF loss. [2] One simple reason is that the surface current has a longer current path. In other words, RF wave energy dissipates excessively due to the radiation loss on the bigger radiation area. This RF loss will contribute into power consumption and aggravate the quality factor. In addition, the electromagnetic field and loss change their locations and values. According to the Ampère's circuit law, the H field integration along the contour on the surface is the same for rough and flat surfaces. However, the loss is proportional to the H2. Thus, due to the least square rule, the total integration of power loss always increases compared to flat surfaces.

Let us consider a 2D random rough surface $Z= f(x)$ in Fig.1. We can expand the magnetic field into Fourier series in x direction. [3]
\[(x,z) = d k_x e^{jk_x x + jk_{1z} z} \sim (k_x) \tag{1}\]

Where \(k_{1z} = \sqrt{k_i^2 - k_x^2}\) and \(k_i\) is the wave number in the superconducting material.

Let us consider how to obtain this wave number in superconductor. According to the two fluid model, there are two types of electrons in a superconducting phase: superconducting and normal conducting electrons. Ohm law in normal conducting material is not applicable in describing superconducting electrons electromagnetic characters. London equations are used to describe the relation of superconducting current density with electric and magnetic fields. They are given in equation 2.

\[
\begin{align*}
\frac{\partial j_s}{\partial t} &= \alpha E \\
\nabla \times j_s &= -\alpha B \\
\alpha &= \frac{n_e e^2}{m} = 5 \times 10^{20} \text{H}^{-1}\cdot\text{m}^{-1} \\
\lambda_s &= \sqrt{\frac{m}{\mu_0 n_s e^2}} = \sqrt{\frac{1}{\mu_0 \alpha}} \tag{2}
\end{align*}
\]

Adapting the London equations into Maxwell equations which are universal valid in both superconducting and normal conducting materials, one can obtain the wave number in side of superconductor in equation 3 (in the gauge \(\text{div}\cdot\mathbf{H}=0\)).
\[ \nabla \times \nabla \times H = \nabla \times (J + \frac{\partial D}{\partial t}) \]
\[ = \nabla \times [(j_s + j_n) + \frac{\varepsilon (i\omega)^2 j_s}{\alpha}]; \quad \frac{j_n}{\sigma_{Normal}} = \frac{i\omega}{\alpha} j_s = E \]
\[ \nabla \times \nabla \times H = \nabla (\nabla \cdot H) - \nabla^2 H \]
\[ -\nabla^2 H = (1 - \frac{\varepsilon \omega^2}{\alpha} + \frac{\sigma_N i\omega}{\alpha}) \nabla \times j_s = -\mu \alpha (1 - \varepsilon \omega^2 \alpha + \frac{\sigma_N i\omega}{\alpha}) H \quad (3) \]
\[ k^2 = -\mu \alpha (1 - \frac{\varepsilon \omega^2}{\alpha} + \frac{i\sigma_N \omega}{\alpha}) \]

We can take the physical property into equation and approximating the wave number. Relative dielectric constant of Nb is 20, the second and third term in the parentheses at 1.5 Ghz is

\[ \varepsilon \varepsilon_0 \omega^2 = \frac{20 \times 8.86 \times 10^{-12} \frac{\varepsilon_m}{m} \times (2\pi \times 1.5 \times 10^9 \frac{1}{s})^2}{5 \times 10^{20} \text{H}^{-1} \cdot \text{m}^{-1}} = 4 \times 10^{-15} \]
\[ i\sigma_N \omega = \frac{250 \times 6.5 \times 10^6 \frac{1}{\Omega_m} \times (2\pi \times 1.5 \times 10^9 \frac{1}{s}) \times i}{5 \times 10^{20} \text{H}^{-1} \cdot \text{m}^{-1}} = 0.03i < i \quad (4) \]

We can infer that 1), at low frequency of 1.5Ghz, the third term in the parentheses is small, and the wave number is pure imaginary, which suggests that electromagnetic wave only sees attenuation and no propagation. 2), at higher frequency of >35Ghz which is Nb de-pairing limit, wave number in the superconductor is $\frac{1-i}{\delta}$, compared with wave number in the normal conductor is $\frac{1-i}{\delta}$. Here $\delta$ is the normal skin depth.

\[ k^2 \square -\mu (\alpha + \sigma_N i\omega) \approx -\mu \alpha = -\frac{1}{\lambda^2} \quad \text{if} \omega \not\approx \omega_{depairing} \quad (5) \]

Now we expand the total magnetic field by FFT into a series of magnetic contributions from each wavelength in spatial frequency.

If we use a second order small perturbation methods, setting

\[ \tilde{H}(k_x) = \tilde{H}^{(0)}(k_x) + \tilde{H}^{(1)}(k_x) + \tilde{H}^{(2)}(k_x) \quad (6) \]

The length of the simulated surface area is up to 2mm which is smaller than the incident electromagnetic wavelength. The magnetic field on the simulated
area can be treated as a fixed constant $H_0$. Thus, the equation above becomes:

$$H_0 = dk_x \exp( jk_x x + jk_t \cdot x f(x)) \sim (k_x)$$  \hspace{1cm} (7)

In this way, the surface magnetic field is redistributed by a Fourier transform to into each surface spatial wavelength in x direction.

By balancing this equation to second order, we obtain the general forms of magnetic field up to second order:

$$\vec{\mu}^{(0)}(k_z) = H_0 \delta(k_z)$$

$$\vec{\mu}^{(1)}(k_z) = -jk_1 H_0 F(k_z)$$

$$\vec{\mu}^{(2)}(k_z) = H_0 \int_{-\infty}^{\infty} dk'_x F(k_z - k'_x) F(k'_x) \left( -k_1 k_x + \frac{k^2}{2} \right)$$ \hspace{1cm} (8)

At this stage, we have calculated the RF magnetic field on this given surface by this small perturbation method. The power absorbed by the conductor, for a given width $w$ in y direction and length $L$ in x direction, can be calculated from the power absorbed by the surface.

$$P_a = \frac{R_s}{2} \text{Re} \int ds \frac{\partial \psi}{\partial n} \cdot \psi^* = \frac{R_s}{2} \int |H(k_x)|^2 ds$$ \hspace{1cm} (9)

By substitute equations 7 into equation 8, we simplify the RF power loss on area $S$:

$$<P_a> = \frac{R_s H^2 S}{2} \left[ 1 + \frac{2r_q^2}{\lambda_L^2} - \frac{2}{\lambda_L^2} \int_{-\infty}^{\infty} dk_x PSD_{1D}(k_x) \text{Re} \sqrt{k_x^2 - k^2} \right]$$ \hspace{1cm} (10)

Note the part outside of the parenthesis is the RF power loss on smooth surface $S$. Remember the square of Root Mean Square (RMS) height, $R_q$ is the integration of PSD within a given frequency as shown in

$$r_q^2 = \int_{-\infty}^{\infty} dk_x PSD_{1D}(k_x)$$

and wave number in superconductor $k_1^2 = \frac{1}{\lambda_L^2}$.

We normalize the power dissipation with that of a smooth surface. We found the power ratio is only related with the surface topography. If the surface is presumed isotropic, we can expand this topographically related power ratio into 2D PSD form.

$$\frac{<P_a>}{P_{a, smooth}} = 1 + \frac{2r_q^2}{\lambda_L^2} \int_{-\infty}^{\infty} dk_\rho PSD_{2D}(k_\rho) \text{Re} \sqrt{\frac{1}{\lambda_L^2} - k_\rho^2}$$ \hspace{1cm} (11)

$PSD_{2D}(k_\rho)$ is the 2D PSD from an isotropic surface and $k_\rho$ is the surface lateral harmonic.
Examining the equation 10, there are 2 important remarks:

1. When third term reduces to $r_q^2 / \lambda_L^2$, when the $k_p$ is small. So the second and third terms exactly cancel each other. Thus, the topographically roughness has no additional RF loss. This means the low frequency surface features contributes no additional loss. However, the sum of the second and third terms only has net contribution if $1/\lambda_L$ and $k_p$ are comparable. The surface feature with lateral length comparable with $\lambda_L$ contributes most additional RF loss.

2. The ratio between $r_q$ and London penetration depth, $r_q / \lambda_L$, is critical for characterizing the increased losses. $\left< r_q^2 \right>_{k_i-\Delta}^{k_i+\Delta}$ in equation 12 denotes the square of RMS height within a $2\Delta$ gap around $k_1$. The Larger $r_q^2$ within this gap produces more additional loss.

$$\frac{\langle P_d \rangle}{P_{d, \text{smooth}}} = 1 + 2 \int_{k_i-\Delta}^{k_i+\Delta} dk_p k_p PSD_{2D}(k_p) \left\{ \frac{1}{\lambda_L^2} - \Re \sqrt{\frac{1}{\lambda_L^2} - k_p^2} \right\}$$

$$= 1 + 2 \int_{k_i-\Delta}^{k_i+\Delta} dk_p k_p PSD_{2D}(k_p) \int_{k_i-\Delta}^{k_i+\Delta} dk_p \left\{ \frac{1}{\lambda_L^2} - \Re \sqrt{\frac{1}{\lambda_L^2} - k_p^2} \right\}$$

$$= 1 + 2 \left< r_q^2 \right>_{k_i-\Delta}^{k_i+\Delta} \int_{k_i-\Delta}^{k_i+\Delta} dk_p \left\{ \frac{1}{\lambda_L^2} - \Re \sqrt{\frac{1}{\lambda_L^2} - k_p^2} \right\}$$

6.3 Application to SRF Surfaces

To obtain more accurate RF loss ratio, one needs to extend the PSD into as broad a frequency range as possible. Since all characterization methods have cut-off frequencies, one can at most get an extended PSD. The recent extended frequency range is $1/1.2$ cm$^{-1}$ ~ $1/10$ nm$^{-1}$, over 6 decades, with white light interferometry and atomic force microscopy. Because the magnetic field is expanded into horizontal spatial wavelength, the PSD frequency should cover the RF wavelength and beyond. Though an approximation method is introduced by using Inverse Abel transforms to extend the PSD frequency range, obtaining 1D PSD with wider frequency range may improve later calculation accuracy. The Abel and inverse transformations are shown in equation 13.

$$\langle W(k_p)^{2D} \rangle = -\frac{1}{\pi} \int_{k_p}^{\infty} \frac{dk_p}{\sqrt{k_p^2 - k_p^2}} \frac{d}{dk_s} \langle W(k_s) \rangle$$

$$\langle W(k_s) \rangle = 2 \int_{k_s}^{\infty} \frac{k_p dk_p}{\sqrt{k_p^2 - k_s^2}} \langle W(k_p)^{2D} \rangle$$

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This transformation also permits the transformation of the high-frequency behavior of the spectra of one dimensionality to be transformed into the high-frequency behavior of the other without knowledge of their low-frequency behavior.

We investigate large/fine/single grain Nb sheets treated by state-of-art polishing methods. Buffered chemical polishing, electropolishing and mechanical centrifugal barrel polishing samples are characterized by Atomic Force Microscopy (AFM) and White light interferometry (WLI). Note that these two characterizations have different lateral resolutions and scan scopes which determine the spectral frequency ranges.

1D averaged PSD is calculated by following the routine introduced previously. [4] Such routine includes proper detrending, windowing and averaging.

In this study, the Rq and PSD are used to derive power ratio. Rq value from 4 different locations on each sample is averaged and summarized in Table 1.

One can generalize that: 1) Rq values from fine grain sheets could be arranged in the decreasing order: BCP>EP>CBP. 2) Fine grain sheets by CBP have larger Rq than large grain sheets. 3) Nanopolished single crystal samples have a larger Rq than the BCP single crystal samples in AFM characterization, but opposite in WLI characterization.

Averaged 1D PSD from AFM/WLI are combined in Fig.2.

After obtained the 2D isotropic PSD, we calculated the Power ratio indexes of these surfaces by equation 10. The indexes are illustrated in Fig.5. Indexes from these surfaces have the power ratio values close to 1.

6.4 Discussion

One can see from power ratio equation that the last term is an integration of 2D PSD.

In equation of power ratio, without the Re(...), the integrand is simply the square of RMS height. One can infer that if the kp is small enough compared with 2/δ, then the Re(...) term reduced into 1/δ. In that limit the second and third terms cancel each other. The total power ratio becomes one. This substantiates the interpretation that features at larger wavelength have less RF power loss than the small high frequency features. Another understanding is that only features with lateral extent comparable to the penetration length give a significant effect on the additional power loss ratio.

Applying this analysis to variously prepared niobium surfaces typical of those in SRF cavities, we find that linear RF losses depend negligibly on roughness for any of the characteristic surfaces considered. On the other hand, SRF materials are particularly susceptible to non-linear and temperature-
dependent losses. The non-linear losses are reflected in the observed Q drop with increasing surface magnetic field. We are examining the influence of topography on such losses separately [5].

One of the advantages of SRF Cavity technology is that the quality factor is much higher than that of the copper cavities. This mainly is because the surface resistance of SRF cavities is much smaller than the surface resistance of conventional normal conducting cavities. This surface resistance reflects the RF power absorbed and consumed on the surface. Due to the superconductivity, magnetic field only penetrates into surface within narrow depth. Thus only thin outer surface layer contributes the most in the RF consumption. Since surface topography is suggested to affects surface resistance, people use several polishing methods to achieve smooth surfaces at reasonable cost. However, there are no definitive trends indicating that the different polishing methods have systematic surface resistance priority than the others in term of cavity Quality factor. This study aims to answer the question how additional power loss attributes to surface roughness by applying the electromagnetic wave scattering theory. This Hyungen scattering method is equivalent to solving Maxwell equation for EM fields.[6] A statistical analysis is given in a form of spectrum to describe surface roughness in the frequency domain. With assumption that surface is isotropic, this 1D spectrum can be expanded into 2D spectrum in order to study the state of art surfaces polishing technologies. A power ratio between a rough surface and a flat surface is given, and this index is only related to surface geometry. Indexes from surfaces with different treatments are compared and discussed in details. There is nonlinearity relation between RF loss and harmonic lateral scale, and one can calculate RF loss with a RF cycle. With characteristic spectrum of each surface treatment, power loss ratio is given at different frequency domains for each treatment.

The 1D PSD curves of differently treated surfaces have a crossover at 1μm. This is mainly because of the grain size. As we claimed before, BCP and EP treatments modify surface differently at intra grain and inter grains scales. BCP treatment polishes the intra grain surface but differentiates the inter grain. On contrary, EP smoothens the inter grain surface but roughens the surface inside a grain. Accordingly, 2D PSD shows a similar trend and the crossover is also at 1μm. Carefully compare the PSD from single crystal and CBP samples; one can see that three types of surfaces have almost the same PSD amplitude beyond 1μm. This means that the CBP technology basically didn't change surface roughness within this range. However, under 1μm frequency, CBPed fine grain has the highest PSD amplitude, and single crystal and CBPed large grain surfaces are almost the same. This suggests that inter grain roughness contributes in this range and CBP could not overcome this inter grain roughness harmonic.
Relating this with the power ratio, even though the ratio index has a small absolute number, we find ratio values follow the same PSD amplitude trend. The ratio indexes have a crossover at frequency 25um\(^{-1}\). The index of EP treated surface remains the same while index of BCP samples increases and reaches peak at 200um\(^{-1}\), then steadily reduces. Indexes from nanopolished surfaces basically decrease, because PSD from this surface at a lateral length comparable to penetration depth has small amplitude and that PSD harmonic at that frequency has a major contribution to RF loss. Other surfaces all show a little peak at frequency 30um\(^{-1}\). These indexes are calculated from the characterization where frequency range may overlap. Another study is promoted and power ratio is calculated from different frequency regions from 2D PSD. Simply take 1um\(^{-1}\) as a boundary.

6.5. Conclusion

The excessive RF power loss from statistical random surface has been analytically calculated by a small perturbation theory. The additional RF loss contribution can be decomposed from each spatial frequency by PSD analysis. Topographically features with different spatial harmonic contribute RF loss differently. The topographical features with the width comparable to London penetration depth dominate the additional RF power loss, their RMS height is critical to the linear RF loss. Meanwhile the features with other spatial frequencies have no net linear RF loss, regardless what RMS height they yield.

Applied to calculate additional RF loss on the surfaces with current surface treatments, this PSD methodology suggests that these surfaces do not yield significant linear RF loss, compared with a flat surface. It is explained that the current surface treatments produce a very small RMS height value on the features with the width comparable to the penetration depth.

6.6 Reference


Fig. 6.1: A plane wave incident impinging on a rough surface with incident angle $\theta_i$.

Fig. 6.2: Joint 1D PSD models from AFM/WLI are shown and the characterization frequency domains are indicated.
Fig. 6.3: Power Ratio calculated from 1D PSD. By inverse Abel transform, the 2D PSD are shown in Fig. 3.

Fig. 6.4: 2D PSD calculated from various surfaces.
Fig. 6.5: Power Ratio by 2D isotropic PSD on the surfaces with the different treatments.
<table>
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<th>Samples</th>
<th>Single crystal</th>
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<tr>
<td>Treatment</td>
<td>After 30 μm BCP</td>
<td>Nano polished</td>
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<tr>
<td></td>
<td>BCP polished</td>
<td>Fine Grain</td>
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<tr>
<td>$R_q$ (nm)</td>
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<td>White light interferometry ~234x312 μm (20x magnification)</td>
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<td>$R_q$ (nm)</td>
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<td>White light interferometry ~930x1244 μm (5x magnification)</td>
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Chapter 7: Superconducting cavity rough surface and interior Magnetic field calculation and explanation of non-linear surface resistance at high field

7.1. Introduction:

It is generally understood that surface roughness can play a role in non-linear RF losses that yield mid-field Q slope and high-field Q drop in niobium-based superconducting radio frequency resonators. [1] In fact, the Q decrease phenomenon is a reflection of increasing averaged surface resistance. Several models attempt to explain the Q slope/drop. Agreement of these models and experiments is mixed. [2]

Typically, BCP treated cavity has Q slope start from 10MV/m to 18MV/m as illustrated in Fig 1. After EP treatment, such high slope is improved up to 24MV/m.[3] This test result suggests that topography evolution plays an important role in improving cavity gradient.

Buffered Chemical Polishing (BCP) treated niobium cavity has Q slope start from 17MV/m to 20MV/m. A very heavily etched cavity evidenced such slope as low as 10 MV/m as illustrated in Fig 1. After electropolishing (EP) treatment, such high slope is improved above 35MV/m.[3] This test result suggests that topography evolution plays an important role in improving cavity gradient.

Even though niobium is a type II superconductor, it has a Ginzburg-Landau factor near the boundary between type I and type II superconductors. In this analysis we treat Nb as a type I superconductor, which has temperature-dependent critical magnetic field Hc. [4] To compare surface roughness, one can use RMS height values (Rq) and power spectral density (PSD). [5,6] Practically, Buffered Chemical Polishing (BCP) treated surfaces, compared to electropolishing (EP) surfaces, have more fluctuations in height and greater density of sharp features. [7] Those high and sharp features enhance the local magnetic field and may exceed Hc. As a result, local superconducting transition is initiated. This amplification may be quantified by a magnetic field enhancement factor (LGMFE). It is a ratio of local magnetic field over background homogeneous excited magnetic field. [8,9,10]

If the local magnetic field is greater than local Hc, flux will enter the surface. As the field decays in depth, magnetic field of some place near the surface must be less than Hc. There may be a stable interface of normal and...
superconducting material. This interface moves inward and outward with frequency of RF. In this equilibrium condition, there will be excessive RF loss due to the normal nucleation sites on the surface. Surface temperature must increase and the local Hc(T) must be reduced. Detailed calculation is needed to evaluate the effective surface resistance, which in turn determines local heat generation. [11] A temperature map must be calculated to estimate the local transition field. This thermal feedback will increase the normal zone area, so iteration is used to approach a stable solution model. In this analysis, we provide a model to calculate nonlinear RF loss from specific microscopic surface topographical features. An averaged surface resistance as a function of H field is given to compare with cavity cold testing experiments.

7.2. Methodology:

7.2.1 Magnetic field calculation:

Electromagnetism:
In order to calculate the electromagnetic field distribution near a rough surface in a resonator with a given RF exciting mode, Maxwell’s equations must be solved with the boundary conditions of this mode.[12] An eigenmode solver is required. We reorganize the Maxwell equation into a Helmholtz wave differential equation as shown below:

\[ (\nabla^2 + k^2)\phi = 0, \quad (1) \]

where \( \phi \) is the magnetic scalar potential and wave vector \( k = |k| = \frac{\omega}{c} \).

After variables separate, space \( \phi(r) \) and time \( T(r) \) always give harmonic general solutions in 1D both as shown below:

\[
\phi(r) = \sum_n C_1 e^{i k_n r} + C_2 e^{-i k_n r} \]

\[
T(r) = \sum_n D_1 e^{i \omega_n r} + D_2 e^{-i \omega_n r} \]

In our case, we simplify the wave equation into a static form near the surface. The simplification is appropriate when the second term in equation 1 is much smaller than the first term. This is applied when the lateral simulation area is much smaller than a wavelength. In our simulation, the lateral scale \( l \) is 100um which is much smaller than the 20cm wavelength \( \lambda \) at 1.5 GHz. At this simulated scale, the k is equal to \( (l / \lambda)^2 \), and it is around 10-10. Therefore, the dominating equation reduces into a Laplace equation.

\[ \nabla^2 \phi = 0, \quad (3) \]
where $\varphi$ is the magnetic scalar potential.
Finite element (FE) or conformal mapping methods can be used to solve the Laplace equation in 2D. Worthwhile noticing, $\varphi$ in equation 2 and 3 can interchange with any electromagnetic field or potential, such as electric field $E$, magnetic field $H$, magnetic flux $B$, magnetic scalar potential $\varphi$ or magnetic vector potential $A$. In this study, we use magnetic scalar potential $\varphi$, which has simple boundary conditions.

We take specific surface profiles from typical fine grain Nb surface preparation and create a simulation model to calculate the local field configuration. Note the surface of typical fine grain niobium with grain size 20-50$\mu$m is reasonably presumed isotropic at scale of 100 $\mu$m. Later, we will calculate RF losses and thermal solutions in which we represent the surface as strips from AFM characterization.

Configuration of Fig.2 illustrates the boundary conditions for magnetic scalar potential $\varphi$ calculation. Dirichlet boundary conditions for boundaries 1 and 3 are given an arbitrary number due to its periodicity. The difference on these two planes determines the amplitude of the magnetic field. The applied field in this analysis is from 80mT to 210mT. Boundary conditions for boundary 2 and 4 are Neumann boundary condition or Perfect Electronic Conductor (PEC) boundary.

From FEM calculation, horizontal lines, in fig .3, are equal magnetic field/flux contours, while the vertical lines are magnetic equipotential contours. Magnetic field at each point of the surface is calculated as a $H_{\text{enhanced}}(x)$ point by point from the finite element calculation. The ratio $H_{\text{enhanced}}(x)/H_{\text{excited}}$ is the Local Geometric Magnetic Field Enhancement (LGMFE) factor. The accuracy of the calculation is related to the surface characterization sampling resolution. However, fine resolution might have too large a data amount to reach affordable computation time efficiency. Note the solution above is a static electromagnetic study, and the time dependence must be added to represent an RF field.

Based on the FEM calculation result, the surface magnetic field is computed by taking the derivative of the scalar potential along the surface, and the resulting LGMF factor is plotted in Fig .4. As shown in Fig.4, the field enhancement factor can vary in the range from 0 to 2 depending on surface topographic 'sharpness.' LGMFE factor is always greater than 1 on surface protrusion, and smaller than 1 on groove areas.
As the applied field is increased, the magnetic fields on some areas of the surface begin to exceed $H_c$. Thus, normal zones begin to nucleate. There would exist a normal and superconducting interface inside the bulk. This interface moves along with RF cycle. The location of this interface is
determined by electromagnetic and thermal configuration and results in effective surface resistance increase. Mathematically, this is known as the Stefan moving boundary problem, and widely simulates surface crystallization process and other phase transition problems. [9] An additional borderline 5 is introduced on Fig 5. It represents the boundary between normal and superconducting materials, called 'normal conducting phase front.' Parallel magnetic field value on this boundary is equal to \( H_c \). The rest of the configuration in Fig 2 remains unchanged. Area between outlines 4 and 5 is normal conductor. Let us introduce how to determine the location of this wave front.

\[
\begin{cases}
  H_\perp = 0 \\
  H_\parallel = H_{\text{critical}} 
\end{cases}
\text{On 5,}
\]

Calculation method:
The basic algorithm to determine this phase front is to iterate to match the known boundary condition which is the parallel \( H \) whose value is \( H_c \) locally. One can start with an actual surface at given magnetic potential and calculate the surface \( H \) field in the vacuum space. If any location on the local surface field has local \( H \) field greater than \( H_{\text{critical}} \), the next step is to reduce this local point's height a certain small amount. Then calculate the field again until the local field is equal to or smaller than \( H_c \). It is a small perturbation theory. Accuracy is reached at expense of vast computing time.

Simulation results and comparison:

Fig.7 represents the results of the calculation of NC/SC phase front deepest penetration at applied \( H \) field values from 80 to 190mT. This deepest penetration moves inward with increasing field amplitude and the interface moves with RF cycle. The blue lines are the deepest penetration that normal zone reaches in each RF cycle. At low field there is no normal zone because the local field is weaker than \( H_c \). For example, if the highest LGMFE is 1.8 and \( H_c \) is 190mT, the normal zone is expected to nucleate at background \( H \) near 115mT.

7.2.2. Thermal simulation and its correction iteration:

Heat equation:
The superconducting state is bounded by three coupled threshold values: current, magnetic field and temperature. Temperature also strongly influences the NC/SC interface location, which in turn determines effective surface resistance. [9] Our thermal calculation uses the results from the
electromagnetism simulation as input. This includes the NC/SC phase front location and H field distributions. The goal for this thermal simulation is to generate a temperature map from the RF surface to the helium bath. As mentioned above, Hc and thermal conductivity are temperature dependent, and superconductivity is lost when temperature is higher than Tc. One needs to calculate a temperature map in order to determine the local Hc, thermal conductivity and subsequent RF loss.

After obtaining a temperature map, one needs to reassign the temperatures back to the material and initiate the next round of temperature simulation because of the thermal conductivity temperature dependency. Such iteration may modify the normal conducting phase front location results from the EM simulation, if the temperature of NC/SC interface is higher than Tc. In this thermal study, another FEM thermal code is developed to calculate the temperatures.

The differential equation for thermal diffusion is:

\[
\frac{\partial T}{\partial t} = \text{div}(\alpha(T)\nabla T) + q
\]

(5)

Where T is temperature, q is related to the internal heat source density, and \( \alpha \) is the thermal diffusivity. Note that this diffusivity is a function of temperature.

Additionally,

\[
q(t, x, y, z) = \frac{Q(t, x, y, z)}{\rho C_p} \quad \text{and} \quad \alpha = \frac{\kappa}{\rho C_p}.
\]

(6)

Where \( \kappa \) is the thermal conductivity, \( \rho \) is density, and \( C_p \) is specific heat capacity, and t is time.

The equation 5 reduces into:

\[
\text{div}(\kappa(T)\nabla T) = \kappa(T)\nabla^2 T + (\nabla T)^2 \frac{\partial \kappa}{\partial T} = Q
\]

(7)

Note the thermal conductivity is also temperature dependent. With rough approximation, the thermal conductivity is a constant because the temperature difference on the surface is small. The equation 7 reduces into a Poisson equation.

\[
\kappa(T)\nabla^2 T = Q
\]

(8)

The last term Q in equation 8 is treated as a dynamic source and the RF power loss at a given field. The thermal diffusion time constant t is determined by \( \frac{\alpha}{\kappa} \), where \( \kappa \) is characteristic size, and \( \alpha \) is the thermal diffusivity, which is 14000 cm-2 sec-1. Therefore, the thermal diffusion time constant is usually at 10-6 second. This means temperature change is a slow change compared with the RF field changes. The Q in equation 8 is an
averaged thermal source, and the temperature map at a equilibrium state is calculated at a given exciting H field. Since the thermal diffusion time is proportional to $i^2$, on the contrary, temperature reacts slowly within the cavity wall where a thermal steady state must exist. The heat equation is the form of equation 8, but the heat source can be treated as an averaged steady RF power within each RF cycle. There must be a transition between these two conditions. In this simulation, the material thickness is 3 mm. If the boundaries are set too small, the simulation leads to temperature calculation error because the side boundaries will need to have heat isolation conditions. However, setting the lateral zone too large costs computation inefficiency. To confidently model the thermal effects from a single small area, the lateral scale in the model needs to be comparable to the material thickness. Thus, the lateral length is 6.6 mm in our simulation. Geometry adaptive meshing is used to adapt to such a high ratio between the thermal simulated area and the scale of surface roughness features. [13]

Boundary conditions are illustrated in Fig 8. Borders 1 and 3 satisfy Neumann boundary conditions. Border 2 is the RF surface. The inset figure is an enlargement of the isolated surface feature with a lateral scale of 100μm located on the center of border 2 with the grey area showing the heat source zone. Convection boundary condition is applied at the border 4. Mathematically, this convection boundary condition is a Robin or absorption boundary condition (ABC): [14]

$$\kappa \frac{\partial T}{\partial n} = h_{Kap}(T - T_{bath}) = \text{Heat flux}$$

(9)

where $\kappa$ is thermal conductivity, and $h_{Kap}$ is Kapitza conductivity between helium and Nb. Both $h_{Kap}$ and $K$ are temperature dependent and given in equation 10. [15]

$$\kappa(T) = 0.7e^{6.57T-0.1T^2}$$

(10)

Next, we consider the heat source term in equation 8. Note that the surface area integration method of equation 11 is applicable only if one presumes uniform conductivity in the volume penetrated by field, which is not valid in our special case. Hence, the RF dissipated amount must be calculated from volume integration, based on the local electric field and electric conductivity.
\[ Q = \int \frac{1}{2} \times R_{\text{surface}} \times H^2 \, dS \quad \text{Non-applicable} \]  
\[ Q = \int \frac{1}{2} \times \sigma \times E^2 \, dV \]  

Here \( R_{\text{surface}} \) is surface resistance and \( \sigma \) is electric conductivity. \( E \) and \( H \) are the surface electric and magnetic field respectively and the integrands are area and volume of the normal zone.

The electric field in the normal zone will be calculated from a quasi-static increasing \( H \) field. From Maxwell--Faraday equation:

\[
\frac{\partial E_x}{\partial y} = \omega \mu h_y \\
\frac{\partial E_y}{\partial x} = -\omega \mu h_x
\]  

where \( e \) and \( h \) are amplitudes of surface electric and magnetic field respectively. \( \omega \) is frequency, and \( \mu \) is permeability of a vacuum. Note, electric field exists only along the \( Z \) axis and its amplitude is integrated by equation 14:

\[
E_z(x, y) = \omega \mu \sin \omega t \left( \int_{y_0}^y -\frac{\partial \phi}{\partial x} \, dx + \int_{x_0}^x \frac{\partial \phi}{\partial y} \, dy \right)
\]  

Electric field \( E_0(x_0, y_0) \) is zero on the phase front, and \( x_0, y_0 \) are the normal and superconducting interface location.

Equation 14 suggests that RF power loss is proportional to \( \omega^2 \). It also presumes that \( E \) is normal to paper plane in this 2D simulation. Power is calculated in the form of discrete power density on each element as an input for the thermal simulation. Compared to the RF loss in the normal zone, the RF loss from the superconducting zone is so small that we neglect it in this stage. This RF loss is the dynamic heat source in equation 8.

To obtain an accurate temperature map inside of the Nb bulk, one needs to update the thermal conductivity locally, then generate a new temperature map until the temperature converges on each element, as illustrated in the flow chart in Fig.9. The RF loss is calculated in terms of effective surface resistance.

Simulation results and comparison:

Using the electromagnetism results described in Fig.7, for applied field amplitude of 100mT, 150mT and 180mT, the results of calculation of the consequent temperature map inside the cavity wall is demonstrated in Fig. 10 for the thermal model of Fig.8.
In Fig.10, the size of heated zones can be as large as sub-mm level. When the excited field increases from 100mT to 120mT, the highest temperature increases from near 94 mK to 300 mK over the helium bath temperature. The temperatures increases nonlinearly with increase of the applied fields.

7.2.3 Electromagnetic and thermal iteration simulation: The big iteration.

The transition Hc of Nb is also temperature dependent. Since the temperature rises at the sharp topographic features, local Hc will also decrease and reconfigure the new electromagnetic field configuration. Thus, we need to introduce a thermal feedback model including the Hc(T) dependency and generate a big iteration on both simulations in section 2.1 and 2.2. Fortunately, Hc varies little at low field, hence this correction is minor. Hc is typically corrected by equation below:

\[ H_c(T) = H_c(0K)[1 - \left(\frac{T}{T_c}\right)^2] \]  

A new SC/NC phase front location is calculated numerically based on a 'big' iteration flow chart, given in Fig. 11.

The flow chart shows a 'big' iteration with two 'small' iterations. EM and thermal iterations were shown in Figs. 6 and 9.

Similar to BCP surface from Fig 2, an EP surface was characterized by AFM and plotted in Fig 12 with the same boundary conditions as in Fig 2. Boundary 4 is the electropolished RF surface with 100μm scan. For all cases, a geometry adaptive meshing is used to address the fine surface features. The inset figure is an enlargement of meshing elements on the center of boundary 4.

The above described integrated analysis was applied to these representative profiles from BCP and EP fine grain niobium surfaces and yields the RF loss increases with applied field shown in Figure 13.

The AFM characterization area covers 100 × 100 μm. The effective raster strip width depends on the sampling rate which, in our case, is 512 × 512. Limited by computational capacity, we reduce the matrix into 32 × 32. Thus, each strip column width is 3.125μm as in Fig.2 and Fig.12. In this analysis, RF losses are integrated from normal zones with width of 3.125μm, and the effective surface resistance is averaged over this strip area which is 100 μm × 3.125μm. A more precise analysis would reduce this strip width.

The indicated increasing RF loss with field is only contributed from the normal conducting zone expansion while ignoring the superconducting losses, and this loss is calculated from equation 12. Fig .13a shows that the
RF losses from individual raster strips and average RF loss from the 32 strips on one AFM image. Fig. 13b gives the relation between RF loss and external field for the sampled BCP and EP treated surfaces.

7.2.4 From topography characterization to surface resistance.

One may next integrate the dissipated power over all of the sampled such strips that make up the representative AFM area scan. This yields the effective RF surface resistance contributed by the induced normal conducting material.

Our previous study has shown statistically that fine grain Nb surfaces have a correlation length which is proportional to the grain size. The correlation length is typically 50μm in this study. In the analysis above, we calculate the RF loss from presumed strip. Further, we need to have adequate strip samples within this correlation length to calculate surface resistance in a given area. As described above, each strip, as the black line shown in Fig. 14, has width of 3.125μm. There are tens of sampling strips within the correlation length.

To calculate the effective surface resistance, we implement equation 11:

To calculate the effective surface resistance, we rewrite equation 11, in which the H field is taken as the exciting field which is homogenous on characterized area S.

\[ R_{surface} = \frac{2Q}{H^2 \int ds} \]

in which the H field is taken as the exciting field which is homogenous on the characterized area S. Meanwhile, the power Q is the loss from normal conducting zones without considering superconducting losses in this stage. We can collect the total RF losses on each strip and calculate the average effective surface resistance on the whole AFM characterized area. Here, we added the superconducting RF loss into the total RF losses. Consequently, surface resistance is comprised of BCS resistance and averaged normal zone resistance. The resulting effective surface resistance is illustrated in Fig. 15.

7.3 Discussion:

7.3.1. Comparison with SRF cavity tests.
So far, the effective surface resistance calculation is derived from a specific characterized sample area. Now we seek to apply these results in a resonant cavity application in order to estimate the quality factor change at different surface H fields. Considering that the local effective surface resistance has field dependency as described above, we integrate the RF loss of a cavity by using equation 16.

\[
P = \frac{1}{2} \times \int_{\text{Cavity}} R(|H|) \times H(r, z)^2 dS(r, z)\]

Taking a rough approximation that the absolute amplitude of surface H field is either zero or maximum along the Z axis of a typical optimized elliptical \(\beta=1\) accelerating cavity [16], we can move the effective surface resistance out of the integrand in equation 16. Thus, the quality factor can be calculated from equation 17.

\[
Q_{\text{topo}}(H) = \frac{\omega_0 U}{P} = \frac{\frac{1}{2} \omega_0 \mu_0 \int H^2 dv}{\frac{1}{2} R_{\text{topo, heat}}(|H|) \times \int_{\text{Surface}} H^2 ds} \cong \frac{G}{R_{\text{topo, heat}}(H)}
\]

A C100 (CEBAF) cavity is simulated in Superfish, and this type of 7-cell cavity is used for the Continuous Electron Beam Accelerator Facility (CEBAF) 12Gev upgrade.[3] The surface H field is illustrated in Fig 16 along the axis direction. In Fig.16, the blue curve is cavity profile while the red curve is surface H field normalized to the peak H field. Thus, in our approximation we can use the geometry factor in equation 17 to calculate Q at given H peak field.

The geometry factor for this structure in this accelerating mode is 280 \(\Omega\). Therefore the Q should be calculated as:

\[
Q_{\text{calc}} = \frac{1}{Q_{\text{BCS}}} + \frac{1}{Q_{\text{topo}}(H)} = \frac{G}{R_{\text{surface, resistance}}(H)} = \frac{G}{R_{\text{BCS}} + R_{\text{heat}}(H)}
\]

where the surface resistance is used from Fig.15. The BCS surface resistance is presumed to have no field-dependency. At 1.5 Ghz, RBCS is \(~13\ n\Omega\) at 2K. Consequently, the Q is dominated by BCS resistance at low field. Fig 17 represents the results of corresponding Q calculation at different of field values.

The quality factor vs peak RF magnetic field curves of BCP/EP treated cavities in Fig.17 qualitatively agree with curves of Fig. 1. Thermal feedback
effects would undoubtedly cause the superconducting surface losses to increase, further degrading the $Q$ beyond that indication by this simulation.

7.3.2. Comparison with excessive topographic RF loss and thermal feedback additional BCS loss.

So far, the analysis ignores the superconducting loss, and this simplification is acceptable if we compare normal zones and superconducting loss in the same area. However, once a normal zone appears, the excessive RF loss will increase the temperature in its proximity, and hence increase the local BCS surface resistance.

As shown in Fig. 10a, the temperature rise on the center of the rough surface may be > 50mK over He bath temperature, and the heated zone has a radius around 0.2mm, which is inversely proportional to local thermal conductivity. This radius is large compared to the normal zone size of several μm as illustrated in Fig 18. Fig. 18 is a top view of the simulated surface. The grey area is the modeled area, the red area is the topographic normal zone, and the blue area is the heated zone where BCS resistance increases due to the temperature positive feedback. We presume there is no additional topographic normal zone within the blue region. As temperature increases from 2K to 2.3K, BCS resistance increases on this heated region by 245%.

Here we calculate additional superconducting loss from the thermal feedback.

If no normal zone is initialized, the whole area is at 2K, where BCS surface resistance is $1.29 \times 10^{-08}$ Ω. Normal zone increases heated region’s temperature to 2.30K at 120mT field amplitude, where BCS resistance is $4.45 \times 10^{-08}$ Ω. Other areas remain at the same temperature of 2K and BCS resistance. A rough approximation shows that the RF loss within the same 100μm × 100 μm area increases from $1.84 \times 10^{-6}$ w to $6.37 \times 10^{-6}$ w when magnetic field value equals ~120mT. The additional BCS loss is $4.52 \times 10^{-6}$ w, and this value can be comparable with normal zone loss $4.34 \times 10^{-5}$ w in Fig. 13 when H field equal to 120mT. The total excessive RF loss related to the normal zone is the sum of these two losses and equals to $4.79 \times 10^{-6}$ w. 91% of this value originates from normal conducting, and 9% belongs to thermal feedback superconducting zone. The percentage of superconducting RF loss as a function of field is listed in table 1. This fraction increases dramatically with H field, and begins to dominate at ~140mT, as superconducting loss is increased due to surface topographic defects. The effective surface resistance will increase accordingly even further. Hence, $Q(H)$ will appear as a steeper drop with increasing H field than that in Fig. 17.
The analysis above is held with the assumption that defective normal zones are isolated. In reality, the heated region zones can affect each other as shown in Fig. 19. The purple area, where two heated regions overlap, has a higher temperature than heated region. Note, the heated region area may differ in size due to the different topographic field enhancement. Thus, the thermal feedback loss induces more RF loss because BCS resistance increases exponentially with temperature. This crosstalk can be solved in the FEM code by iterating temperature between two 2D stripes calculation till the temperature converge.

7.3.3. Comparison with cavities internal surface characterization.

As mentioned above, the effective non-linear surface resistance induced by surface topography is related to the density of normal zones. These normal zones are initialized due to the topographic geometry field enhancement. Therefore, in order to achieve a better predictive capability, we need to characterize statistically representative sample areas for further analysis. In surface characterization, roughness features are observed by AFM technology. White Light Interferometry (WLI) allows one to increase the characterization scale. Two typical practical surfaces obtained by the WLI technique are shown in Fig. 20. The scan parameters were given in previous reports [13, 14]. Increased confidence in the representative character of the above analysis would come from applying the same methodology to the large scale data sets.

One can see from Fig. 20.a that the BCP surface has island-like features, and the edges of these features have possibility to be normal zone ignitions. EP treated surface in Fig. 20.b is much smoother and does not have many sharp edges. The density of possible normal zones on EP sample is less than BCP sample, and the effective surface non-linear resistance is consequently smaller.

7.4. Conclusion:

Electromagnetic and thermal simulations were conducted to obtain a microscopic normal and superconductivity conductor phase front based on specific topography and applied field. This phase front is a function of exciting magnetic field, and this interface determines the normal zone areas which in turn contribute significantly in the RF power loss. Each normal zone initiates its expansion based on the local geometric field enhancement factor. With a certain electromagnetic field applied, a temperature map is obtained. More accurate normal zone phase front modeling is obtained with considering critical field temperature dependency. Normal zone on the surface expands nonlinearly with increasing external magnetic field. Such
nonlinearity can be represented in the form of effective non-linear surface resistance. Additional superconducting RF loss is induced as a result of thermal feedback. The total RF power loss contribution thus induced solely by topographic roughness may be calculated in this manner. Initial results of this analysis using representative topographic profile data from typical etched and electropolished fine grain niobium surfaces yield a nonlinear loss character and Q dependence with field which are quite similar to that typically observed with L-band SRF accelerating cavities with the corresponding surface treatments.

7.5. Reference.

Performance of HG006 with initial light electropolishing treatment.

Fig. 7.1: A typical Q-E curve of cavity with BCP and sequent EP treatments.

Fig. 7.2: Configuration used for simulation model calculation. A cross section fragment of the real BCP treated sample surface. Area in blue represents vacuum volume. Borderlines 1 and 3 determine the exciting magnetic field. Borderline 2 is Perfect Electric Conductor (PEC) and border 4 outlines a BCP treated surface profile, also PEC, acquired by AFM scanning.
Fig. 7.3: Magnetic scalar potential solution in Laplace equation. The vertical dot lines are magnetic equipotential contours. Horizontal lines are magnetic field lines.
Fig. 7.4: The Local Geometric Magnetic Field Enhancement factor (LGMFE) map is calculated from profile in Fig 2.
Fig. 7.5: Configuration used for simulation model calculation. A cross section fragment of the real BCP treated sample surface. Area in blue represents vacuum volume. Borderlines 1 and 3 determine the exciting magnetic field. Borderline 2 is PEC. Additional border 5 which outlines an interface of normal and superconducting materials is introduced and also is PEC.
Calculate the magnet field on actual surface profile (FEM)

**NO**

Field along the surface? > Threshold transition field \( H_c \)

\[ \text{YES} \]

Continue on next surface

Reduce the local coordinates downwards by 0.1%, reconstruct a new surface

Fig. 7.6: Flow chart to determine the free NC/SC boundary and calculate the field configuration in the vacuum.

![Flow chart](image)

- Actual surface
  - Interface with field
    1. 100mT
    2. 150mT
    3. 180mT

Fig. 7.7: Normal conducting phase fronts are calculated from excited fields list in table 1.

![Graph](image)
Fig. 7.8: Typical temperature simulation area in 2 dimensions: Borders are labeled in number. Grey area represents internal heat source location and borders 2 and 4 are RF surface and Helium interface respectively.
Initial condition: presume conductivity is uniform @2k and add the external heat from previous electromagnetism NC/SC boundary

Solve the Poisson equation and obtain Temperature map1

Resign both conductivities corresponding to Previous T map,
Solve the Poisson equation and obtain Temperature map2.

If Tmap1 - Tmap2 < Tolerance

YES

Calculation halts and render Temperature map.

Fig 7.9: The flow chart of thermal equation simulation.
Fig 7.10: Temperature maps are calculated at excited magnetic field of 120 and 190mT. The simulated surface has a lateral scale of 100μm in Fig .2.
Boundary condition: \( H_{\text{perpendicular}} = H_{\text{sh}}(T) \) on NC phase front.

Thermal conductivity \( T \) in bulk. Kapitza \( T \) at the Helium Boundary.

1. EM determined NC/SC interface.
2. EM field E/H configuration.

Electromagnetism simulation

Output: 1. Temperature map.
2. Integrated and discrete RF Power dissipation on elements.

Thermal Temperature simulation

Fig. 7.11: Flow chart of Electromagnetic and Temperature simulations.
Fig. 7.12: Boundaries are labeled in number. Area in blue represents vacuum, and boundary 4 is the surface characterized by AFM from a practical EP treated sample. Boundaries 1 and 3 determine that exciting field and boundaries 2 and 4 are PEC. The above described integrated analysis was applied to these representative profiles from BCP and EP fine grain niobium surfaces and yields the RF losses increase with applied field shown in Figure 13.
Fig. 7.13a: Total power dissipation on a 3.125μm wide strip due to representative topographic roughness as a function of peak macro H field. Superconducting losses are ignored.
Fig. 7.13b: BCP stripe calculation and averaged. Total power dissipation on a 3.125µm wide strip due to representative topographic roughness as a function of peak macro H field. Superconducting losses are ignored.

Fig. 7.14: AFM images from a fine grain niobium sample with a) about 100µm removal by BCP, b) after electropolished at 30 °C to remove 48 µm. Horizontal scale is 20 µm per division and vertical scale is 5 µm per division.[5]
Fig. 7.15: Effective RF surface resistance with peak H field of two different surfaces. Topography alone makes the difference.

Fig. 7.16: Surface magnetic field is illustrated on CEBAF 7-cell cavity from Superfish simulation.
Fig. 7.17: Comparison of the calculated cavity quality factor of two different surfaces at different peak H fields, without consideration for thermal feedback on superconducting material.

Fig. 7.18: Surface temperature distribution top view. The grey area is the characterized area, the red area is normal zone from topography, and the blue area is the heat affected zone. The center line is 2D stripe used in section 2.1.
Fig. 7.19: Surface temperature distribution top view. The grey area is the characterized area, the red area is normal zone from topography, and the blue area is the heat affected zones. The purple area is an area where two HEATED REGION overlap. The counterstrike lines are 2D stripes used in section 2.1.

Fig. 7.20: Typical niobium polycrystalline surfaces characterized by white light Interferometer after BCP (left) and additional 30um off EP (right) treatments.
Table 7.1: The temperature, RBCS, Super/normal conducting RF loss and its percentage are shown as a function of different H fields. The normal conducting loss is sum of RF loss from all strips in Fig.13a.

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Appendix A
Matlab program (GUI) for Power spectral density for surface roughness.

From folders on the left, open “compile PSD”, then “0. Workable PSD for PP”, double click “interface.m”, click run of F5.
Click “Setup”, change length of scan (unit in nm), change order if needed (the larger area scanned, the higher order should be used).

If you need to manually adjust the length and resolution, please change it in the boxes next. Do the same if you want to change the order of detrending and windows function.

Click “calculate”, choose an original AFM file from the pop-up window.

PSD will import image, calculate 1D PSD and detrended surface.
The RMS from figure and PSD integration is shown in the indication boxes.
Click "save report" on the right hand side, word will pop-up. However, if need 2D PSD, click "calculate 1D to 2D" instead, you will see the bar on the top is moving.
Once press calculate 2d PSD, one 1D PSD fitting figure is popped out.

1D PSD fitting is coming out.
Click "save report if yellow" on the right hand side, a MS word is coming and save.

To plot PSD, from Matlab "File" click "import data", choose file from folder, data will imported into Matlab. The doc and Matlab data will be saved in the same directory where AFM/WLI data is from. The directory is shown on the top of console. (MS WORD 2010 need some changes.)

Click reset for a next round. Click "running" if want to add another image on existing PSD plot.
IF you want to plot PSD in another figure in Matlab.

File  Edit  View  Debug  Parallel  File

New  Open...  Close Current Folder  Import Data...  Save Workspace As...  Set Path...
          Ctrl+O  Ctrl+W
Preferences...

Ctrl+P
Look in:

- Recent Places
- Desktop
- Libraries
- Computer
- Network

Name:...
Date modified:...
Type:...

File name:

Files of type: Recognized Data Files

Select variables to import using checkboxes

- Create variables matching preview:
  Create vectors from each column using column names.
  Create vectors from each row using row names.

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<tr>
<td>y</td>
<td>512</td>
</tr>
</tbody>
</table>

Type in command

\[ \text{loglog}(\text{PSD}(1,:),\text{PSD}(2,:)); \]
Use "hold on" if plotting in Matlab for plotting multi PSD on one plot, while you can do multiple time of this to plot PSDs in one figure to compare. A legend and axis labels will be added by clicking view>plot Brower.
Read the output MS word doc, information will be explored from there. They are in publication format.
Appendix B:

A Matlab program (with GUI) to calculate fine electromagnetic field on sub micron surface features.

Here, AFM picture is shown.

The power dissipation is shown in this box.

A cartoon of normal zone growth will be popped in another window.

Finite element methods (FEM):

```
%function []=fem_50_2 (height32)
load height32
data=height32;
for number=1:length(data)
    newheight(number,1)=real(data(number));
    newheight(number,2)=imag(data(number));
end
x=newheight(:,1);
y=newheight(:,2);
node=[x,y]
```

% here we could refine the mesh
cd('H:\12.1 self FEM2dmesh\Mesh2d v24\')

%set(0,'DefaultFigureVisible','off')
[p t]=mesh2d(node);
%set(0,'DefaultFigureVisible','on')

%triplot(dt);
disp('total number=')
length(p)
disp('total face=')
length(t)
%p is the vertex coordination.

[p,t] = refine(p,t);
[p,t] = refine(p,t);
%[p,t] = refine(p,t);
cd('H:\12.1 self FEM\fem50\')
coordinates=p;
save coordinates.dat p -ascii
elements3=t;
save elements3.dat t -ascii

%save elements3.dat elements3.dat32

%boundary condition
%1 dirichlet.data
% surface (1-68)and excitation (69-70)
edgenode=transpose(tableup(node,p));

cd('H:\12.1 self FEM\iso2mesh\')
faceedge=volface(elements3);
facenodes=unique(faceedge(:,));
cd('H:\12.1 self FEM\fem50\')

%edgeline=findedge(coordinates(facenodes,:),coordinates(edgenode,:));
edgeline=findedge(coordinates(faceedge(:,1,:),coordinates(edgenode,:));
% This is the BC Definition: very important
% start with easy oneseither NBC or DBC.
ii=1;
for i=1:length(edgeline)
    if edgeline(i)>=d1 & edgeline(i)<=d2
        dirichlet(ii,:)=faceedge(i,:);
        ii=ii+1;
    end
end
dirichlet1=dirichlet;
for i=1:length(edgeline)
    if edgeline(i)>=d3 & edgeline(i)<=d4
        dirichlet(ii,:)=faceedge(i,:);
        ii=ii+1;
    end
end
dirichlet2=unique(dirichlet);

if n1>n2
    n2=n2+length(data);
end

if n3>n4
    n4=n4+length(data);
end
jj=1;
for i=1:length(edgeline)
    if edgeline(i)>=n1 & edgeline(i)<=n2
        neumann(jj,:)=faceedge(i,:);
        jj=jj+1;
    end
end

if n1>n2
    n2=n2+length(data);
end

if n3>n4
    n4=n4+length(data);
end
jj=1;
for i=1:length(edgeline)
    if edgeline(i)>=n1 & edgeline(i)<=n2
        neumann(jj,:)=faceedge(i,:);
        jj=jj+1;
    end
end

%2 neumann.data
% surface (68-69)and excitation (70-1)
neumann1=neumann;
for i=1:length(edgeline)
    if edgeline(i)>=n3 & edgeline(i)<=n4
        neumann(jj,:)=faceedge(i,:);
        jj=jj+1;
end

for k=1:length(neumann)
    j=j+1;
    if neumann(j,1) ==0
        if neumann(j,2) ==0
            neumann(j,:)=Q;
            j=j-1;
        end
    end
end
save neumann.dat neumann -ascii

for k=1:length(dirichlet)
    j=j+1;
    if dirichlet(j,1) ==0
        if dirichlet(j,2) ==0
            dirichlet(j,:)=Q;
            j=j-1;
        end
    end
end
save dirichlet.dat dirichlet -ascii

%%% FEM_50 applies the finite element method to Laplace's equation.
%
% Discussion:
FEM_50 is a set of MATLAB routines to apply the finite element method to solving Laplace's equation in an arbitrary region, using about 50 lines of MATLAB code.

FEM_50 is partly a demonstration, to show how little it takes to implement the finite element method (at least using every possible MATLAB shortcut.) The user supplies datafiles that specify the geometry of the region and its arrangement into triangular and quadrilateral elements, and the location and type of the boundary conditions, which can be any mixture of Neumann and Dirichlet.

The unknown state variable U(x,y) is assumed to satisfy Laplace's equation:

- \( U_{xx}(x,y) + U_{yy}(x,y) = F(x,y) \) in \( \Omega \)

with Dirichlet boundary conditions

\( U(x,y) = U_D(x,y) \) on \( \Gamma_D \)

and Neumann boundary conditions on the outward normal derivative:

\( U_n(x,y) = G(x,y) \) on \( \Gamma_N \)

If \( \Gamma \) designates the boundary of the region \( \Omega \), then we presume that

\( \Gamma = \Gamma_D + \Gamma_N \)

but the user is free to determine which boundary conditions to apply. Note, however, that the problem will generally be singular unless at least one Dirichlet boundary condition is specified.

The code uses piecewise linear basis functions for triangular elements, and piecewise isoparametric bilinear basis functions for quadrilateral elements.

The user is required to supply a number of data files and MATLAB functions that specify the location of nodes, the grouping of nodes into elements, the location and value of boundary conditions, and the right hand side function in Laplace's equation. Note that the fact that the geometry is completely up to the user means that just about any two dimensional region can be handled, with arbitrary shape, including holes and islands.

Reference:

Jochen Alberty, Carsten Carstensen, Stefan Funken,
Remarks Around 50 Lines of MATLAB:
% Short Finite Element Implementation,
% Numerical Algorithms,
% Read the nodal coordinate data file.
% load coordinates.dat;
%
% Read the triangular element data file.
% load elements3.dat;
%
% Read the quadrilateral element data file.
% load elements4.dat;
%
% Read the Neumann boundary condition data file.
% I THINK the purpose of the EVAL command is to create an empty
% NEUMANN array
% if no Neumann file is found.
% eval ('load neumann.dat;', 'neumann=[];');
%
% Read the Dirichlet boundary condition data file.
%
load dirichlet.dat;

% all facenodes are the boundary nodes, but unknown to DBC or NBC.
% more important, faceedge are the boundary edge to refine DBC AND
% NBC.

% NOW WE ARE REVISING BCs.

A = sparse ( size(coordinates,1), size(coordinates,1) );
T = sparse ( size(coordinates,1), size(coordinates,1) );
b = sparse ( size(coordinates,1), 1 );
%
% Assembly.
%
for j = 1 : size(elements3,1)
A(elements3(j,:),elements3(j,:)) = A(elements3(j,:),elements3(j,:)) ...
   + stima3(coordinates(elements3(j,:,:),));
end

% for j = 1 : size(elements4,1)
%   A(elements4(j,:),elements4(j,:)) = A(elements4(j,:),elements4(j,:)) ...
%      + stima4(coordinates(elements4(j,:)));
% end
%

%%
load 3d512 %things unchanged
   data11=to32line(data);
   %data11=height32;
   dataline=data11(aii,:);
for number=1:length(dataline)-2
   newheight1(number,1)=real(dataline(number));
   newheight1(number,2)=imag(dataline(number));
end
xx=newheight1(:,1);
yy=newheight1(:,2);
orginal = fit(xx,yy,'linearinterp');
%
%% T matrix
clear i

k1=1.5e9*6.28/(3e8*1e9);%in vacuum
%k1=0.00005;

k2=i*4*3.14e-7*6.6e6*1.3e9*6.28/1e9;% in normal bulk already k2^2
%k2=k1;
for j = 1 : size(elements3,1)
   if sum(coordinates(elements3(j,:),2))/3 >
      orginal(sum(coordinates(elements3(j,:),1))/3) %center above then vacuum
      T(elements3(j,:),elements3(j,:)) = T(elements3(j,:),elements3(j,:)) ...
      + k1^2*Tstima3(coordinates(elements3(j,:,:),));
   else %center below then in normal bulk
      T(elements3(j,:),elements3(j,:)) = T(elements3(j,:),elements3(j,:)) ...
      + k2*Tstima3(coordinates(elements3(j,:,:)));
   end
end
% Volume Forces.
for j = 1:size(elements3,1)
    b(elements3(j,:)) = b(elements3(j,:)) + det([1,1,1; coordinates(elements3(j,:));']) * ...
    f(sum(coordinates(elements3(j,:)))/3)/6;
end

% for j = 1:size(elements4,1)
%     b(elements4(j,:)) = b(elements4(j,:)) + ...
%     det([1,1,1; coordinates(elements4(j,1:3));'] ) * ...
%     f(sum(coordinates(elements4(j,:)))/4)/4;
% end

% Neumann conditions.
% if (isempty(neumann))
%     for j = 1:size(neumann,1)
%         b(neumann(j,:)) = b(neumann(j,:)) + ...
%             norm(coordinates(neumann(j,1),:) - coordinates(neumann(j,2),:)) * ...
%             g(sum(coordinates(neumann(j,:)))/2)/2;
%     end
% end

% Determine which nodes are associated with Dirichlet conditions.
% Assign the corresponding entries of U, and adjust the right hand side.
% u = sparse(size(coordinates,1), 1);

BoundNodes = unique(dirichlet);

% % % % % % % % % % % % % % % % % % % % % % % % % % % %
% [cii cib](phiii; phiib)-[tii tib](phiii; phiib)=0 or =-[tii tib](fii; fib)
% [cii cib](phiii; phiib)-[tii tib](phiii; phiib)=0
% [cii cib](phiii; phiib)-[tii tib](phiii; phiib)=0
% [cii*phiib+phiib=tii*phiib+tib*phiib;
% % [cii*phiib-tii=phiib-cib*phiib;
% % (cii-tii)*phiib=(tib-cib)*phiib;
%here this is phi = magnetic scalar potential.
%the magnetic field is gradient phi.
% the distance is 104um.
% for the critical phi = 104 * e-6(meter) * 2000 (oe)
% while 2000 oe= 80*2000=160000 A/m.
% now phi = 104 * e-6 (meter) * 160000 (A/m)=16 (Ampere).
% the unit for later field should be ampere and should devide 10e e-6
% (meter)
middle = u_d (coordinates,coordinates(BoundNodes,:),edgenode,d1,d2,d3,d4,excitedfield);

for i=1:length(BoundNodes)
u(BoundNodes(i)) = middle(i);
end

%based on the boundnode, the u(boundnode) should be the Dirichlet BC.
b = b - A * u + T * u;
%
% Compute the solution by solving A * U = B for the remaining unknown
% values of U.
% FreeNodes = setdiff ( 1:size(coordinates,1), BoundNodes );

% u(FreeNodes) = A(FreeNodes,FreeNodes) \ b(FreeNodes);
u(FreeNodes) = (A(FreeNodes,FreeNodes)-T(FreeNodes,FreeNodes)) \ b(FreeNodes);
%
% Graphic representation.
%
%u=real(u);

show ( elements3, coordinates, full ( u ) );

return

%end
Appendix C
A Matlab program to calculate temperature on sub micron surface features by using the output from Appendix B.
Finite element methods to heat equation:

```matlab
function fem_50_heat ()

%% FEM_50_HEAT applies the finite element method to the heat equation.
%
% Reference:
% % Jochen Alberty, Carsten Carstensen, Stefan Funken,
% % Remarks Around 50 Lines of MATLAB:
% % Short Finite Element Implementation,
% % Numerical Algorithms,
% % Volume 20, pages 117-137, 1999.
%
% Local Parameters:
% % Local, real DT, the size of a single time step.
% % Local, integer NT, the number of time steps to take.
% % Local, real T, the current time.
% % Local, real T_FINAL, the final time.
% % Local, real T_START, the initial time.
% %
timestamp()

cd('H:\14.Thermal feedback\fem50 heat\poisson static\')
%
% Read the nodal coordinate data file.
% load coordinates.txt;
%
% Read the triangular element data file.
% load elements3.txt;
% p=coordinates;

t=elements3;
```
% Read the Neumann boundary condition data file.
% I THINK the purpose of the EVAL command is to create an empty NEUMANN array
% if no Neumann file is found.
% eval( 'load neumann.txt;', 'neumann=[];'
%)
%
% Read the Dirichlet boundary condition data file.
% There must be at least one Dirichlet boundary condition.
% load dirichlet.txt;
% load robin.txt;
%
% Determine the bound and free nodes.
% load edgenode.txt
%
A = sparse ( size(coordinates,1), size(coordinates,1) );
b = sparse ( size(coordinates,1), 1 );
%
% Assembly.
%
u = sparse ( size(elements3,1), 1 );
load thermal_diffusivity.mat
for j = 1 : size(elements3,1)
    % diffusivity = conductivity/density/specific heat;
    % density = ;
    % specific heat = ;
    % density*specific heat = heat capacity;
    % for ii = 1:length(elements3Q, :)
        centerT = 1/3*(u(elements3(j, 1)) + u(elements3(j, 2)) + u(elements3Q(ii, 3)));
        % conductivity = exp(1.65*centerT - 0.1*centerT^2)*0.7; % unit W/(K*m)
        % usually 10~1000
        % conductivity1 = conductivity*1e-9; % change unit into W/(K*nm);
        % usually 1e-8;
        % alpha = conductivity;
    % if centerT < 300,
        % alpha = 0.0001;
    % else

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% diffusivity = thermal_diffusivity1(centerT)/10000;
% if diffusivity < 0.0001
% alpah = 0.0001;
% else
% diffusivity = 0.7 * exp(1.65 * u(ii) - 0.1 * u(ii).^2);
% alpha = diffusivity;
% end
% end

conductivity = thermal_diffusivity(centerT); % unit W/(K*m) usually 10^-1000

% alpha = diffusivity * 1e-9 * 3125; % change unit into W/(K*nm); usually 1e-8;
alpha = conductivity * 1e-9; % change unit into W/(K*nm); usually 1e-8;

A(elements3(j,:), elements3(j,:)) = A(elements3(j,:), elements3(j,:)) +
stima3(coordinates(elements3(j,:),:));
A(elements3(j,:), elements3(j,:)) = A(elements3(j,:), elements3(j,:)) +
alpha * stima3(coordinates(elements3(j,:),:));

end

%% APPLY Robin BC:
if isempty(robin) ~= 1

%% robin BC can still change the K stiffness matrix.
robinmatrix = [1/3, 1/6; 1/6, 1/3];

% for j = 1 : size(robin, 1)
value = abcrbin ( robin(j,:), t, coordinates, edgenode, u );
A(robin(j,:), robin(j,:)) = A(robin(j,:), robin(j,:)) - ...
norm(coordinates(robin(j,1), :) - coordinates(robin(j,2), :)) *
robinmatrix * value(2);
end
%
% Robin conditions change Mass vector b.
% for j = 1 : size(robin, 1)
value = abcrbin ( robin(j,:), t, coordinates, edgenode, u );
b(robin(j,:)) = b(robin(j,:)) - ...
norm(coordinates(robin(j,1), :) - coordinates(robin(j,2), :)) * ...
value(1)/2;
end
end
% Volume Forces.
% 
load shortdataformat.mat
heightreal32=data11(aii,:);
load finalboundaries.mat
finalboundary=finalboundaries{aii,excitedfield};
% [a,b]=size(finalboundaries);
% for ii=1:c
% finalboundary(ii)=finalboundaries(aii,excitedfield,ii);
% end
for jj=2:length(finalboundary)-3
    finalboundary123(jj)=finalboundary(jj);
    heightreal32123(jj)=heightreal32(jj);
end
finialboundaryfunction=fit(real(finalboundary123(:)),imag(finalboundary123(:)),'linearinterp');
heightreal32function=fit(real(heightreal32123(:)),imag(heightreal32123(:)),'linearinterp');
iiii=1;
external=[,]; % where the heat is applied, external is heat element number coordinates.
for j = 1 : size(elements3,1)
    xy=sum(coordinates(elements3(j,:),:))/3;
    if xy(2)>finialboundaryfunction(xy(1)) & xy(2)<heightreal32function(xy(1))
        external(iii,1:2)=sum(coordinates(elements3(j,:),:))/3;
        external(iii,3)=j; % record which element it labeled.
        iii=iiii+1;
    end
end
% field distribution:
load Epower.mat
heat=Epower{aii,excitedfield};
[Efieldfitresult, gof] = Efieldfit(heat(:,1),heat(:,2),heat(:,3));
%
wrongtime=0;
righttime=0;
fitnan=[];
fitgood=[];

totalpowermid=0;
totalareas=0;
for j = 1 : size(external,1)
    %b(elements3(j,:)) = b(elements3(j,:)) ... 
    % + det( [1,1,1; coordinates(elements3(j,:))'] ) * f1(sum(coordinates(elements3(j,:)))/3,aii,excitedfield)/6;
    aaa=f1(external(j,1:2),Efieldfitresult);
    if isnan(aaa)~=1
        b(elements3(external(j,3,:))) = b(elements3(external(j,3,:))) ... 
        + det( [1,1,1; coordinates(elements3(external(j,3,:))')] ) * ... 
        aaa/6;
        totalareas=totalareas+det( [1,1,1; coordinates(elements3(external(j,3,:))')] ) * aaa/2;
    else
        wrongtime=wrongtime+1;
        j;
        fitnan(wrongtime)=j;
        end
    end
    righttime=righttime+1;
    j;
    fitgood(righttime)=j;
else
    wrongtime=wrongtime+1;
    j;
    fitnan(wrongtime)=j;
end
end
totalpower(aii,excitedfield)=totalpowermid/totalareas;
avchen(1)=totalpowermid;
avchen(2)=totalpower(aii,excitedfield);
%aii=1;
%excitedfield=1;
% plot heat source
% if isempty(fitnan)&isempty(fitgood)
% %% display em NC/SC boundary Tc line and actual surface
% %aii=1;
% %excitedfield=1; %%%%please change here!!!
%
% excitedfield=excitedfield+1;
% load finalboundaries.mat;
EMfinalboundaries=finalboundaries{aii,excitedfield};
plot(EMfinalboundaries,'r'); hold on;
% load height32.mat; plot(height32,'b'); hold on;
% load Epower.mat; chenchenpower=Epower(aii,excitedfield);
plot(chenchenpower(:,1),chenchenpower(:,2),'b*'); hold on;
% axis([-10000 100000 -50000 50000]);

% Neumann conditions.
%
% for j = 1 : size(neumann,1)
%     b(neumann(j,:)) = b(neumann(j,:)) + ...
%         norm(coordinates(neumann(j,1,:)) - coordinates(neumann(j,2,:))) * ...
%         g ( sum(coordinates(neumann(j,:,:))/2, t,coordinates,edgenode ) / 2;
% end
%
% Determine which nodes are associated with Dirichlet conditions.
% Assign the corresponding entries of U, and adjust the right hand side.
%
% % Robin Boundary condition.

u = sparse ( size(coordinates,1), 1 );
%
%% apply dirichlet boundary condition, if no Dirichlet then simple initial u.
BoundNodes = unique ( dirichlet );
if isempty(BoundNodes)~=1
    u(BoundNodes) = u_d ( coordinates(BoundNodes,:));
end
b = b - A * u;
%
% Compute the solution by solving A * U = B for the remaining unknown values of U.
%
FreeNodes = setdiff ( 1:size(coordinates,1), BoundNodes );

u(FreeNodes) = A(FreeNodes,FreeNodes) \ b(FreeNodes);

%show ( elements3, coordinates, U, nt, t_start, t_final );
%set(0,'DefaultFigureVisible','on')
%axis auto
u=u*1000; %change the Kelvin into miliKelvin;
set(0,'DefaultFigureVisible','off')

%show ( elements3,coordinates,full ( u ),excitedfield);
%plot(full(u),'DisplayName','u','YDataSource','u');figure(gcf);

%

% Terminate.
%
fprintf ( 1, '
');
fprintf ( 1, 'FEM_50:
');
fprintf ( 1, ' Normal end of execution.
');
fprintf ( 1, ' Normal end of execution.
');

xlabel('Lateral width (nm)');
ylabel('Cavity wall thickness (nm)');
zlabel('Temperature Map (mK)');

% timestamp ( );

return
Appendix D
A Matlab program to calculate 2D PSD from 1D PSD with half inverse Abel transformation.

```matlab
%PSD

%m1234=createFitm1234(x,y)
lowerlimit=15000000;
resolution=800;
x2d=linspace(1/lowerlimit, 1/100, resolution);

deltaX= (1/100-1/lowerlimit)/resolution;
y2d=zeros(1,length(x2d));
for i=1:length(x2d)
    y2d(i)=myintegral(m1234,x2d(i));
end

y2d=abs(y2d);
psd2d=[x2d;y2d];

%plot (x2d,y2d);
%rms=quad(m123,1/(234000), 1/490);

rms1 = sqrt(1/640*quad(m1234,3.215434083601286e-06, 0.001027326149845));

%%rms from 2d psd
rms2=0;
clear i
for i=1:length(y2d)
    %y2d is already 2d PSD;
    rms1(i)=deltaX*y2d(i)*deltaX;
    rms2=rms2+rms1(i);
end
rms2=sqrt(rms2)/12.8;

%%

%rms1=integrate(m123,0.001023495333119,4.273504273504274e-06);
%plot (x,yy);
skindepth=40;
sum=0;
clear i
kprime=sqrt(-(2*i/skindepth^2)-x2d.^2);
for i=1:length(y2d)
```

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%y2d is already 2d PSD;
sum1(i)=x2d(i)*y2d(i)*real(kprime(i))*deltaX;
sumtotal=sumtotal+sum1(i);
end
pratio=1+2*(rq(data)/skindepth)^2-4*3.14/skindepth*sumtotal;
pp=pratio/lowerlimit;
Autobiography

Chen Xu was born in Beijing on April 17th 1983. He received his B.A in Electronic Engineering in Materials science department in Fudan University in Shanghai in July 2005. After that he was admitted to Ph.D program in the material science and engineering department of Tsinghua University in Beijing. In August 2007, he entered the Applied science department of the college of William and Mary. With the completion of the thesis and satisfaction in all other degree requirements, Chen Xu is expected his Ph.D degree in Applied Science in Feb 2013.

Awards:

- Tsinghua University Scholarship 2006/2007
- Samsung Scholarship first class 2003
- Fudan University People Fellowship Scholarship 2004/2005.
- William and Mary Research/Travel Grant 2012/2013
- Best Student awards in International Particle accelerator conference 2012.
- Student Poster awards top5 Linac international conference 2012.
- 2012 Chinese National Merit Scholarship for students.

First Author Journal Review Paper:

3. Analysis of high field non-linear losses on SRF surfaces due to specific topographic roughness (Accepted by Applied surface science in Nov 2012)
4. SRF cavity surface topography characterization using replica techniques (submitted to Supercond Sci Technol in Dec 2012)
5. Surface impedance study on rough surface by Fourier Harmonic simulation by RF wave reflection and adsorption theory. (submitted to Rev. ST Accel. Beams in Dec 2012)