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Modeling, Fabrication, and Optimization of Niobium Cavities – Final Phase

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**TRP Research Area:** Accelerator / Transmutation Sciences

**Budget Request:** $161,147
Abstract
Niobium cavities are important parts of the integrated NC/SC high-power linacs. Over the years, researchers in several countries have tested various cavity shapes. They concluded that elliptically shaped cells are the most appropriate shape for superconducting cavities. The need for very clean surfaces lead to the use of a buffered chemical polishing produce for surface cleaning to get good performance of the cavities. This is the third and final phase of the study. The first phase has resulted in improving the basic understanding of multipacting and the process of chemical etching. The second phase has resulted in an experimental setup of a fluid flow experiment with experimentation to be completed in the third year. Other experimental activities include the evaluation of a vacuum system and various vacuum equipment purchases and modifications. An optimization code for a five cell niobium cavity based on resonant frequency and mode number was developed. Based on our conclusions so far, as well as our interaction with personnel at Los Alamos National Laboratory (LANL), we propose to focus on the following topics in the third phase of this project:
1. Optimize the cavity shape based on the desired resonant frequency and examine multipacting of that structure.
2. Studying secondary electronic emission from a niobium test piece under cryogenic conditions.
3. Experimental study of the etching process using flow visualization techniques.
4. Redesign the etching process to maximize surface uniformity.

Introduction
The nuclear industry provides a significant percentage of the world, including the United States, with electricity. Nuclear power plants produce thousands of tons of spent fuel. Some of this spent fuel can be radioactive for thousands of years. The US DOE is currently exploring the possibility of creating a permanent storage site at Yucca Mountain, Nevada for nuclear spent fuel. Accelerator Transmutation of Waste is one complementary approach to deal with spent nuclear fuel. In this approach, a particle accelerator produces protons that react with a heavy metal target to produce neutrons. These neutrons are used to transmute long-lived radioactive isotopes into shorter-lived isotopes that are easier to be handled. A major component of the system is a linear accelerator (linac) that can accelerate a 100-mA beam of protons up to 1 GeV [1]. Los Alamos National Laboratory (LANL) is an active participant in developing a superconducting rf (SCRF) high-current linear accelerator. SCRF has three major components: niobium cavities, power couplers, and cryomodules. This proposal mainly deals with niobium cavities.
Niobium cavities have several advantages including small power dissipation compared to normal conducting copper cavities. These cavities are usually made of multiple elliptical cells. Refer to Figure 1. They are formed from sheet metal using various techniques such as deep drawing or spinning. The cells then are welded using electron-beams. Multi-cell units are usually tuned by stretching or squeezing them. Niobium cavities need very clean surfaces, which can be achieved by chemical polishing and high pressure rinsing with ultra-pure water.
Figure 1. Schematic Diagram of Niobium Cavities (Executive Summary: Development and Performance of Medium-Beta Superconducting Cavities (LANL))

Under operation very high electromagnetic fields are present in these cavities. Besides the intended acceleration of a particle beam, these fields can also accelerate electrons emitted from the niobium surfaces. An electron emitted from the surface of the cavity wall is guided and accelerated by these RF-fields until it impacts on the cavity surface again. This re-impact can lead to the generation of one or more secondary electrons that in turn act as primary electrons that possibly might generate more electrons in a localized region. The number of secondary electrons is determined by the impact energy of the electron and by the secondary emission coefficient of the cavity material. If secondary electrons are created in phase with the RF-fields, and the impact is localized, a rapidly rising multiplication of electrons will occur. This localized resonant process is known as multipacting (multiple impacting). As a consequence, RF power is absorbed and it becomes impossible to increase the cavity fields by raising the incident power. The electron collisions with the structure walls lead to a temperature rise and eventually to a breakdown of the superconductivity. As a result, the $Q_0$ (quality factor) of the cavity is significantly reduced at the multipacting thresholds. Also, structural damage of the surface can occur. A good cavity design should be able to eliminate, or at least minimize multipacting. The factors that affect multipacting include: shape, surface finish, and coating.

While models have been suggested for minimizing multipacting [2], practical means of manufacturing the cavity walls to obtain optimal designs are still an issue. Attempting to improve the performance of multiple niobium cavities may be a daunting task because of the computational load associated with the evaluation of a particular design and the large number of variables and constraints involved. We propose approaching this task in a systematic way using principles of nonlinear programming. The consequence of this effort will allow the Superconducting RF Engineering Development and Demonstration group at LANL and the faculty at UNLV to target potential cavity cell configurations that improve upon existing designs.

Summary of Achievements of Phases I and II:

1. **Optimization of the shape of the cavity to produce the desired resonant frequency and mode of operation**: This is a unique study with no precedent in the available literature. We have created a framework for interacting with two dimensional field codes
developed by Field Precision Inc. and an optimization program within a MATLAB environment. Figure 2a illustrates the outcome of a seed geometry, Fig. 2b, as the optimization routine hones in on the target frequency (700 MHz) and mode (pi mode). It is to be noted that the optimization process was stopped after a few days of iteration. At the time the code was terminated, the resonant frequency was approaching the target 700 MHz frequency but the pi mode was not found. It is observed that as the end cavities and the end pipes terminating the five cell geometry approach the same radius, both the target resonant frequency and the pi mode constraint will be found but for a three cavity geometry system as compared to the five cavity system. This implies that the optimization code is properly converging but it is converging to a geometry that is not of interest. The cavity geometry currently being employed at the LANL is illustrated in Fig. 2c. The end cells of the seed geometry (Fig. 2b) differ significantly from the existing geometry (Fig. 2c). The optimization process is being further constrained so to converge on a more desirable solution.

(a) Five-cell niobium cavity approaching an optimized geometry

(b) Five-cell niobium cavity seed geometry
2. Assessment of a vacuum chamber and assembly to be used for SEE from niobium test piece. An existing vacuum chamber has been modified for SEE studies. Through various donations, a cryogenic pump with controller was obtained. The vacuum chamber has been tested by an independent company to determine its capability to hold ultra low vacuum. It has been determined that pressures to $10^{-9}$ Torr should be possible. An electron gun, heat tape, and a RGA are on order. To save about $55,000 or more, the insides of an old cryogenic pump is being used as a cryostat. The “cryostat” was tested by the manufacturer and will reach superconducting temperatures for niobium ($\sim 8 \, ^{\circ}\text{K}$). Quotes for a manipulator and load-lock chamber have been obtained. Figure 3 shows the existing cavity with pumps and blanks.

3. Assessment of current etching techniques presently used in LANL: The current method uses a baffle to direct the etching fluid toward the surface of the cavity. Refer to Figure 4. Finite element analysis shows that the baffle partially succeeded in achieving its purpose as can be seen in Figure 5. The flow is however restricted to the right half of the cavity with very limited circulation in the left half, which results in more etching of the iris region compared to that of the equator regions. These results confirm the observations of [3]. The current design also experiences flow circulation behind the baffles in the second through fifth cavity cells. There is a significant increase in velocity at the outlet.
4. **Optimization of the Baffle Design:** An alternative design is proposed and modeled. The proposed baffle design is also modified so that it can be extended inside the cells of the cavity. The exit flow is now parallel to flow inlet, Figure 6. Results show that flow circulation is eliminated. The flow is now closer to the surface of the cavity. We used optimization techniques to improve this design. [16]
Figure 6. Velocity Field for the Optimized Modified Baffle Design

5. **Experimental Visualization of the Verification of the Etching Process**: LANL has loaned us a transparent cavity for use in flow visualization, Figure 7. A transparent plexiglass box was manufactured to enclose the cavity. Pump and piping system were also modeled, Figure 8. A complete setup including a computer-controlled x-y traverse and digital camera was assembled, Figure 9. We are currently testing the setup.

Figure 7. Photo of the LANL Transparent Cavity
6. These research activities are disseminated through:
   • One paper that was presented in the International Congress on Advanced Nuclear Power Plants (ICAPP), Hollywood, Florida, June 2002. The title of the paper is, “Modeling and Optimization of the Chemical Etching Process in Niobium Cavities.”
   • Discussions with LANL personnel, especially Dr. Tsuyoshi Tajima.
**Research Objectives**

The research objectives are:

1. Continue current research on the phenomenon of multipacting.
2. Optimize the shape of the cavity based on the desired resonant frequency and mode and examine multipacting properties.
3. Experimentally study of secondary electron emission from a niobium piece (1 cm$^2$) that has been surface-conditioned by LANL.
4. Use the flow visualization experimental setup to evaluate flow patterns of the etching fluid inside a plastic model of the niobium cavity with various baffle designs.
5. Redesign the etching process to maximize surface uniformity by considering the effects of rotating the baffle within the cavity.

**Technical Impact**

The proposed work will make a major contribution to the understanding and design of niobium cavities. This area is very critical with many recent developments, e.g. [4], [5], and [6]. The proposed research will provide a means to benchmark the codes for LANL specific objectives. To our knowledge, few if any studies have examined secondary electron emission of niobium in the superconducting state. It is believed that the physics of the material is far different in this state as compared to that at room temperature. Also, empirical data obtained from experiments will be incorporated into the Track_RF code. The proposed research will result in a method for optimal design of superconducting RF-resonators. Our research is multi-disciplinary, combining expertise from three distinct areas (electromagnetics, fluid dynamics, and optimization). Graduate students involved in this project will be exposed to these three areas and will be expected to work as a team. It is expected that this interaction will result in several publications gaining recognition of UNLV activities in this area as well as attracting additional funds to the university.

It is anticipated that the developed modeling tool will impact the efficiency of future superconducting cavity designs of interest to the Superconducting RF Engineering Development and Demonstration (SRFEDD) group at LANL and elsewhere. Such a study will guide the (SRFEDD) group and their UNLV collaborators to establish fabrication strategies for manufacturing. These efforts should also lay the foundation for examining multipacting in RF windows in the future.

**Research Approach**

The proposed research can be divided into several interconnected tasks as shown in Figure 10. The remainder of this section details our approach to each task.
Task 1. Multipacting

Numerical models of multipacting are of great interest for the design of RF cavities for high energy proton accelerators. Multipacting is a resonant phenomena of an electron avalanche as a result of localized impact due to secondary electron emission. The growth of a localized current originating and terminating on the cavity wall absorbs and dissipates a part of the electromagnetic energy stored in the cavity. Multipacting lowers the $Q_0$ of the cavity limiting the energy stored by the cavity. It can also cause damage to the RF-surface. By conditioning the cavity (operating the RF cavity at its highest achievable field level in the absence of the beam), soft barrier healing of the cavity may be possible lowering the secondary emission coefficient. This may be a time intensive process. The shape of the cavity structure, its material composition, and the surface treatment play significant roles in mitigating multipacting processes. It has been shown that cavities with a more circular wall geometry along the cavity axis inhibits multipacting relative to elliptical cavities, [7]. The SEE (Secondary Electron Emission) curve for niobium at room temperature is well known. Even so, multipacting is dependent of the surface treatment of the cavity. Different niobium surface treatments can alter the SEE coefficient by nearly a factor of three, [8]. This is significant since niobium has a maximum SEE coefficient of 1.1 at an electron impact energy of about 500 eV. Further, the surface treatments examined in 1986, [8], are not necessarily the same types of treatments currently used on superconducting cavities at LANL. Moreover, it is known that surface kinetics plays a significant role in the secondary emission. Besides the impact energy, also the impact angle may have to be considered for proper modeling, [9]. In practice, the niobium cavities are operated at cryogenic temperatures yielding a superconducting state. Little to no information is readily available on the SEE in this state. It is anticipated that the SEE coefficient will be different than that at room temperature. This is because the physics of superconductors at cryogenic temperatures dictates that the electric force on charges is only balanced only by their inertia since charge collisions within the material are negligible to zero. Therefore, as an electron approaches the superconducting material, conduction electrons will be Coulomb repelled within the material away from the point of impact. Secondary electrons emitted from the site of impact may require more energy to be emitted from the surface as a result compared to room temperature niobium. It is therefore of interest to study the niobium material in the state similar to that in the accelerator.
It is proposed to study the SEE from the surface of niobium samples treated at LANL at cryogenic temperatures in a superconducting or near superconducting state. In a test, an electron beam, generated from an electron gun source, will impinge with both normal and oblique incidence on the sample surface now termed as the target. It is intended that the target be of a spherical (hemispherical) geometry held at various negative potentials relative to a set of collecting anode segments surrounding the target. With proper potential adjustments, ampere meters will be used to measure the primary current at the target and the secondary currents at the segmented anode plates. Information on the SEE trajectories, distribution and amount is to be determined by the study. Figure 11 illustrates a typical experimental setup. A highly sensitive current amplifier with an extremely low current sensitive switching network

Figure 11. Typical SEE (Secondary Electron Emission) experimental setup with detailed circuit for sensor array.
will be used to amplify and convert the current signals to measurable voltage signals. The target under test must be held at cryogenic temperatures in a vacuum environment; \(10^{-8}\) to \(10^{-9}\) Torr. Studying the distribution of the SEE will give a clue on how to statistically handle changes in the grain structure of the material. Experimental conditions similar to that in RF superconducting cavities are sought.

Experimental data will be fit to generic theoretical curves (Refer to Figure 12) whenever possible and used in computational multipacting studies currently being developed at UNLV based on 2D codes provided to us from Field Precision.

Based on [9], it is anticipated that some of the experimental data sets may not follow accepted theoretical predictions as the angle of incidence changes even when the incident beam is far from the grazing angle. It is anticipated that new results will be obtained with our experimental setup. The literature does not appear to contain experimental studies on the angular distribution of the scattered secondary electrons emitted from a surface treated sample relative to the incident angle of the primary electron beam. Further, SEE from a sample in a superconducting state does not appear to be readily available.

**Task 2: Optimal Design of Niobium Cavities for a Desired Resonant Frequency**

Phase II of the project resulted in optimizing the design of the outermost cell of the niobium cavity to produced a desired resonant frequency. The objective function that was used is:

\[
\text{minimize} \left| \frac{700MHz - \omega_0}{700MHz} \right|
\]

where, \(\omega_0\) is the angular frequency of the accelerating mode. The problem is subjected to dimensional constraints as described in Figure 13. These constraints are:
\begin{align*}
A_1 & \leq y_a + r_a \leq B_1 \\
A_2 & \leq x_c + L_a \leq B_2 \\
A_3 & \leq y_c - b_c \leq B_3 \\
A_4 & \leq x_c \leq B_4 \\
A_5 & \leq \frac{a_c}{b_c} \leq B_5 \\
A_6 & \leq r_a \leq B_6 \\
A_7 & \leq \phi_a \leq B_7 \\
A_8 & \leq \phi_L \leq B_8 \\
\end{align*}

The optimization algorithm used in this problem is Fuzzy Simplex [13], which incorporates fuzzy logic to make the simplex search flexible. Results, Figures 2a-c, show that the optimization search radically modified the design of the cell. The next stage is to incorporate the inner cells into the process. Similar set of constraints will be added to represent these cells. The final design will be assessed to ensure that multipacting is minimized.

There are a number of criteria that need to be considered, when optimizing niobium cavities. The most important ones are the quality factor, \( Q_0 \) [2] and the ratios of peak surface fields to the average accelerating field in the cavity. As a first step in optimizing the niobium cavities the quality factor is used as a performance measure. It is defined as

\[
Q_0 = \frac{\omega_0 U}{P_c}
\]

where, \( U \) is the stored energy and \( P_c \) is the power both dissipated in the cavity walls and absorbed by the multipacting electrons, and \( \omega_0 \) is the angular frequency of the accelerating mode. The peak field ratios will be considered according to a strategy that will be defined in collaboration with LANL. The above equation shows that minimizing the lost energy and maximizing the stored energy can maximize the quality factor. An alternative measure of multipacting used is the global multipacting factor, [11], which is the averaging over the total number of initially emitted electrons over the distributed cavity surface,

\[
N_0 \prod_{m=1}^{k} \delta(K_m)
\]

Because we are optimizing the geometry of the cavity to reduce or eliminate multipacting, the above measure will be modified to monitor multipacting at localized regions on the cavity surface. To take into consideration that secondary electrons may be responsible for initiating multipacting, a number of particles with varying phase will be launched at positions where the secondary electron emission is greater than unity. This will allow us to artificially track secondary electrons that may potentially cause multipacting.
Figure 13. Variables that Describe the Cavity

Task 3: Optimal Design of the Etching Process
The ultimate goal of the primary optimization is a cavity shape that fulfills all mechanical and RF requirements. The optimization of the chemical etching will be conducted for this cavity design. The velocity of the flow should be as uniform as possible in the case of laminar flow to ensure a uniform etching. Velocity distribution will allow mass transfer rates to be calculated to determine etching rates of the surface.

Task 4: Redesign the Etching Process to Maximize Surface Uniformity
The surface finish of the niobium cavity plays an important role for achieving the best performance. Even microscopic contaminants on the surface of the cavity can seriously affect its performance due to magnetic heating or electron field emission. As a consequence, a surface finish treatment is needed after fabrication of the cavity. Studies in the first phase of this project using computational fluid dynamics (CFD) helped in better understanding the process. Our preliminary studies also showed that the quality of etching could be further improved. We propose to look at several questions during this phase of the project including:

1. Redesign of the Baffle
2. Study the effect of turbulence on etching
3. Flow visualization

The remainder of this section details the proposed approach for these subtasks.

4.1. Redesign of the Baffle:
As seen in an earlier section, we already started the process of redesigning the baffle. The new design results in a more laminar flow (Figure 6) which may be achieved by extending the
baffle inside the cavities. Design of an expanding baffle represents a challenging problem due to space limitations and the chemically aggressive environment. Figure 14 and Figure 15 represent possible designs for the baffle. The first one has differing geometry that the existing one while the other design is cam-activated one that can be expanded within the cavity. We will be designing and manufacturing several prototypes during this phase of the project.

![Figure 14. Possible Design for Static Baffle](image)

a. Retracted Baffle  b. Expanded Baffle

![Figure 15. Possible Design for an Expanding Baffle](image)
4.2. Flow visualization:

Flow visualization is needed to help verify the FEA simulations and to give better insight into the problem. During this year we incorporated a transparent plastic cavity that LANL loaned us into an experimental setup to simulate different etching conditions. Refer to Figure 16. Previous numerical work produced velocity distributions within the etchant used to produce the final finish in the niobium cavities. The flow is laminar and pockets of recirculating flow were reduced by changing the baffle design. Instead of performing verification of the predicted velocity distributions on a prototype niobium cavity using acid etchant at great expense, we will be choosing a “model” fluid that has the same Reynolds number for the desired flowrate. The velocity of the “model” fluid is adjusted for differences in fluid density and viscosity:

\[
V_m = V_p \left( \frac{\rho_p}{\rho_m} \right) \left( \frac{D_p}{D_m} \right) \left( \frac{\mu_m}{\mu_p} \right)
\]

In this expression, the subscripts for the model (m) and prototype (p) system are related through dimension, D, density, \(\rho\), and dynamic viscosity, \(\mu\).

Experiments are proposed using a flow visualization technique to visualize the flow of a “model” fluid through a plastic prototype of the niobium cavity provided by LANL. Dye injection will be used to verify that the numerical codes accurately predict the flow behavior seen in the experimental model system. Dye injection provides quantitative verification that laminar flow exists within the niobium cavities during etching. It can also verify the absence of recirculation pockets within the cavities. Several factors will be considered including, different flow rates and flow patterns, i.e. laminar or turbulent flows, with or without agitators or baffles.

Figure 16. Front View and Side View of Baffle in Flow Visualization Experiment

4.3. Study the effect of turbulence on etching:

Finite element simulation shows that the current etching configuration results in a fluid flow that is at the borderline between laminar and turbulent flow. No research has considered the effect of turbulence on chemical etching. The flow can be made turbulent by rotating the baffle. This process may however be restricted by practical consideration of limited baffle rotational velocity. Previous discussions with LANL personnel indicated that the baffle may have a
rotational speed of 10 rps. CFD simulation of the process will be conducted to assess the usefulness of turbulent flow.

**Capabilities at the University and Los Alamos:**

LANL is already active in the area of designing SCRF cavities. Lab personnel have collaborated with US industry in the area of cavity fabrication. Some of the research facilities needed to pursue this project are available at UNLV.

**Equipment Requested for AAA User Labs:**

- **Secondary Electron Emission Experiment:** A switching network is required to minimized the number of ampmeters and current amplifiers needed to measure the currents resulting from secondary electron emission. The currents generated as a result of SEE will be very small and need to be amplified. A special current amplifier is needed for the study. In order to move the niobium piece under test *in situ*, a manipulator arm with load-lock chamber is needed. The following hardware is needed for implementing SEE experiments: flanges and pipe connections, high voltage feed-throughs, overall clean-up and maintenance cost, pressure gauges, materials for building electrode system, cryogenic feed-throughs.
- **CFD simulation of chemical etching:** We are using FEMLAB (plus Chemical Engineering Module) and MATLAB for this purpose. We have licenses for one year. Software licenses will need to be updated.
- **Redesign of the Baffle:** Materials are required for creating different prototypes.
- **Flow Visualization:** Dyes and seeding particles are needed in support of fluid flow experiments. Additional equipment such as pumps, pipes, and fittings may be needed if the experimental setup is to be modified.

**Project Timeline:**

**Timeline Narrative**

The proposed research is planned to cover one year, starting in Summer 2003. Research will be conducted with close interaction with appropriate personnel at LANL.

**Expected Technical Results:**

- Secondary Electron Emission results for niobium material.
- Optimization code based on the resonant frequency of the cavity and pi mode operation.
- New baffle design.
- Flow visualization in modeled cavity structure.

**Milestones (Based on starting date of May 15th, 2003)**

- Have a working optimization code based on the cavity resonance. September 2003
- Complete fluid flow experiments. September 2003
- Ordered most of the vacuum equipment and assemble vacuum system. September 2003
- Finish thesis on fluid flow studies December 2003
• Complete SEE experiments February 2004
• Incorporate SEE results in multipacting code. May 2004
• Complete thesis on SEE by May 2004.

Note: Researchers will produce quarterly progress reports to help monitor the progress of the project.

Deliverables
In addition to the quarterly and final reports, researchers expect to publish the results of this project at the appropriate technical conferences and journals. This project will lead to M.S. theses for the graduate students participating in this project. Final report due April 2004.

References
Appendix: A. Copy of Support Letter from Dr. Tsuyoshi Tajima, Team Leader Accelerator Physics & Engineering LANSCE-1, LANL

Main Identity

From: "Tsuyoshi Tajima" <tajima@lanl.gov>
To: Robert A. Schill, Jr. <schill@ee.unlv.edu>
Cc: "Mohamed B Trebia" <mbt@me.unlv.edu>
Sent: Thursday, February 27, 2003 2:03 PM
Subject: RE: Niobium Cavity Proposal - Final Phase

Bob and Mohamed,

I am about to leave the lab and will be going to England for a week from tomorrow (2/28-3/7).
I don't think I can send you a letter by noon tomorrow, but try to send you an email or fax sometime next week.

Tsuyoshi

----Original Message-----
From: Robert A. Schill, Jr. [mailto:schill@ee.unlv.edu]
Sent: Thursday, February 27, 2003 2:46 PM
To: Tsuyoshi Tajima
Cc: Mohamed B Trebia
Subject: Niobium Cavity Proposal - Final Phase

Tsuyoshi,

We are in the process of completing the final draft of the proposal for funding in the third and final year. We would like your input in the proposal as well as a letter of support for the research. Unfortunately, we must submit the proposal tomorrow. Sorry for the short time frame on this. Both Mohamed, the students, and myself have been working long hours trying to complete as much work as possible before submission of this effort. The first section of the proposal shows some of the work completed over the past one and three-fourths years. This will be of interest to you. The remainder of the proposal is what we intend to do. We are missing a picture and some minor updates at this time.

If it is possible and if you feel that the effort is worthy of future support, we would appreciate a letter of support from you. If we do not receive this by noon tomorrow (Friday 2/27/03), we will submit the proposal and indicate that a letter of support may follow next week.

We hope all is well with you and appreciate your interest in our work. If you have any questions or comments, please contact either myself or Mohamed.

Best wishes,

Bob Schill, Jr.

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