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Modeling, Fabrication, and Optimization of Niobium Cavities: Phase I

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Date: April 13, 2001
Refer to: AAA-TPO-01-038

Dr. Mohamed B. Trabia
Dr. Robert A. Schill, Jr.
Department of Mechanical Engineering
University of Las Vegas
4505 Maryland Parkway
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Dear Drs. Schill and Trabia:

Subject: Proposal for Modeling, Fabrication and Optimization of Niobium Cavities

I have received your proposal on superconducting (SC) RF cavity development, "Modeling, Fabrication, and Optimization of Niobium Cavities." The proposed research fit well with the SC RF development work that is ongoing in the AAA Project. It is the recommendation of a recent review by the AAA External Review Committee that the ADTF Linac will be all-superconducting except for the 6.7-MeV RFQ. Such recommendations greatly increase the importance and relevance of your proposal.

Your proposed development of computation techniques to understand cavity shapes and chemical processing will be beneficial to the Project and the SCRF community. It will identify paths for improving cavity performance. It will help in early identification and resolution of difficulties before the actual fabrication of cavities leading to cost saving.

I wholeheartedly support your proposal and wish you success. My support will mainly be in consultation and as the liaison between you and the AAA ED&D on SCRF Linac.

Yours Sincerely,

K. C. Dominic Chan
SCRF ED&D
Project Leader

Cy:
APT/TPO File

Project Title: Modeling, Fabrication, and Optimization of Niobium Cavities – Phase I

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AAA Research Area: Accelerators / Transmuter

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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 and buffered chemical polishing produce good performance. The objective of the proposed research is to maximize the performance of the niobium cavities through studying multipacting, studying the effect of chemical etching on the surface roughness, and redesigning the cavities.

Introduction

Nuclear industry provides a significant percentage of the world, as well as that of the United States, 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. The US Congress has recently authorized exploring an alternative way to deal with spent nuclear fuel: Accelerator Transmuting of Waste (ATW). In this approach, a particle accelerator produces protons that react with a heavy metal target to produce neutrons. A major component of the system is a linear accelerator (linac) that can accelerate over 100 mA of protons to several GeV [1]. Los Alamos National Laboratory (LANL) is currently 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.

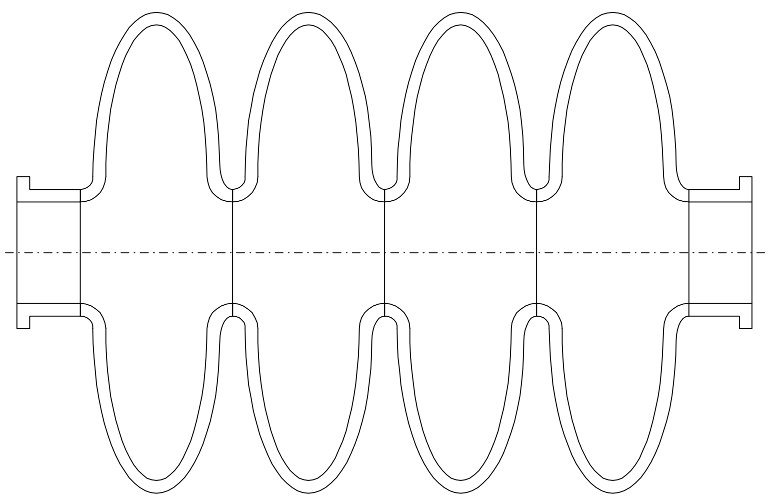

Figure 1. Schematic Diagram of Niobium Cavities

Niobium cavities have several advantages including small power dissipation compared to normal conducting copper cavities. These cavities are usually made of multiple elliptical cells, 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. The niobium cavities are chemically polished and then subjected to high pressure rinsing.

Under operation, an electron emitted from the surface of the cavity wall is guided and accelerated by the RF fields supported by the cavity until impacting with the wall occurs. This leads to the generation of a large number of secondary electrons that in turn act as primary electrons to generate more electrons in a localized region. This localized resonant process is known as *multipacting*. As a consequence, RF power is absorbed such that it becomes impossible to increase the cavity fields by raising the incident power. The electrons collide with the structure walls leading to a large temperature rise and eventually to superconducting cavities, thermal breakdown. As a result, the Q_0 (quality factor) of the cavity is significantly reduced at the multipacting thresholds. A good cavity design should be able to eliminate, or at least to minimize, multipacting. The factors that affect the 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 is still an issue. For example, acid used to smooth the surface of the cavity walls does not necessarily etch the surface uniformly. This in turn affects the wall geometry, the fields supported by the cavity, and hence its multipacting properties.

Attempting to improve the performance of multiple niobium cavities may be a daunting task because of the computational load associated with evaluating 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 Engineering Accelerator Group at UNLV to target potential cavity cell configurations that improve upon existing designs.

Research Objectives

The research objectives are:

- To study the effect of multipacting on niobium cavities with single and multiple cells.
- To improve the uniformity of surface finish in chemical etching.
- To investigate the relationship between the shape and surface condition of the cell and its performance.
- To provide a systematic approach for improving the performance of the niobium cavities.

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. [3] and [4]. Existing two dimensional multipacting codes will be used to examine a means of enhancing science based understanding of the multipacting loss mechanism and mitigating this loss mechanism resulting from cavity design flaws in manufacturing. Computational fluid dynamics will be used to produce a better method for producing a smooth uniform surface in chemical etching. The results of both areas will be combined to propose a method for optimal design of the unit. The proposed research is multi-disciplinary that combines 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 thedeveloped modeling tool will impact the efficiency of future superconducting cavity design of interest to the Superconducting RF Engineering Development and Demonstration (SrfEDD) group at LANL. Although more efficient designs are of paramount importance, the maximum degree of error allowed in the fabrication of the cavity walls will be considered. Such a study will guide the (SrfEDD) group and their UNLV collaborators to in establishing required fabrication strategies for manufacturing. These efforts should also lay down the foundation for examining RF window multipacting in the future.

Research Approach

The proposed research can be divided into three tasks: multipacting in niobium cavities, study of ways to improve uniformity of chemical etching, and optimal design of niobium cavities. These three tasks are interconnected, Figure 2. The remainder of this section details our approach to each task.

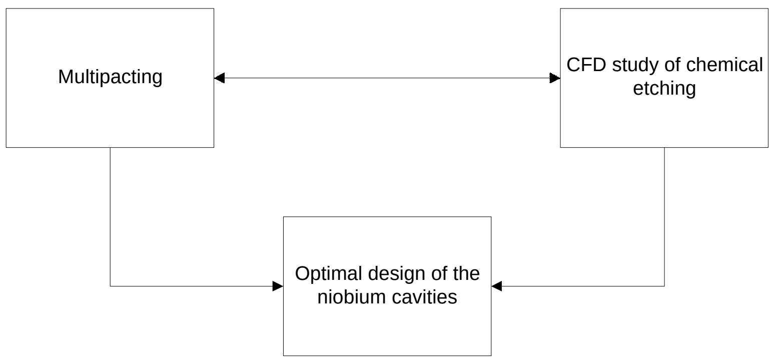

Figure 2. Research Tasks

Task 1. Multipacting

The accepted mechanism of multipacting is as follows. A primary electron, emitted from the surface of the cavity or structure, is accelerated by the RF fields and eventually impacts the surface of the container. Secondary electrons are generated as a result of the impact. These secondaries are in turn accelerated, impact the wall and generate more electrons. More and more electrons are generated resulting in an avalanche type of effect. The process continues but eventually saturates due to space charge effects and available RF power.

Impacting is therefore material and geometry dependent. The geometry of the cavity determines the field structure and the distribution of the RF power the cavity supports. The number of new electrons emitted is dependent on the secondary emission coefficient. This is material related which depends on the impact energy of the primary electron.

Generally, it has been shown that one-point multipacting will occur in regions where the magnetic field along the cavity wall does not vary significantly and where stable trajectories are possible. Past studies have indicated [5] that spherical cavity geometry tends to destroy the resonance property of multipacting. The magnetic field varies along the surface of the wall such that there are no stable electron trajectories. In practice, elliptical shaped cavities are employed due to improved mechanical stability and easy drainage of liquids during the manufacturing process, [6].

Two-point multipacting occurs when impacting electrons resonate between two spatial locations in the cavity. Typically in an elliptical cavity this results on two sides of the equator of the ellipse. The starting energy is usually low for β *(=v/c) =1* cavities. Consequently, careful manufacturing of the cavity surface tends to eliminate this resonance.

Although models have been developed to guide one in minimizing multipacting [2], practical means of manufacturing the cavity walls to obtain optimal designs is an issue. Ways to minimize multipacting include localizing the regions where multipacting is most eminent as a consequence of manufacturing flaws and redesign the wall geometry with wall perturbations conducive to manufacturing processes that will minimize multipacting. Another alternative is to examine other choices of materials or material composites with lower secondary emission coefficients (SEC) or SEC, which have significant electron emission only over a narrow impact energy range. In this case one can allow for high energy and low energy electron impacting with a probable level of assurance that multipacting may not be significant. In all cases, careful controlled manufacturing of the cavity is imperative. Contaminants or surface imperfections alter the field geometry supported by the cavity and tend to initiate impacting, which may lead to multipacting due to the thermal breakdown (melting) at a localized point. In many cases, this is also used as a means of conditioning the cavity at points where multipacting results. Another novel technique is to locate points of multipacting based on their thermal signatures on the cavity surface while under operation and use some form of in situ controlled laser processing to perturb the cavity wall so to minimize impacting.

A two-dimensional Field Precision code (Track_RF), [7], will be in part purchased and employed to study multipacting in geometries exhibiting azimuthal symmetry. This finite element code will be employed to first reproduce common one-point and two-point multipacting scenarios. The software can model the effects of beam-generated electric and magnetic fields, automatic generation of input distributions, self-consistent space-charge-limited emission, and field emission. Trak requires the TriComp mesh generator and Estat, Bstat, and WaveSim to prepare electric and magnetic field input files, Figure 3.

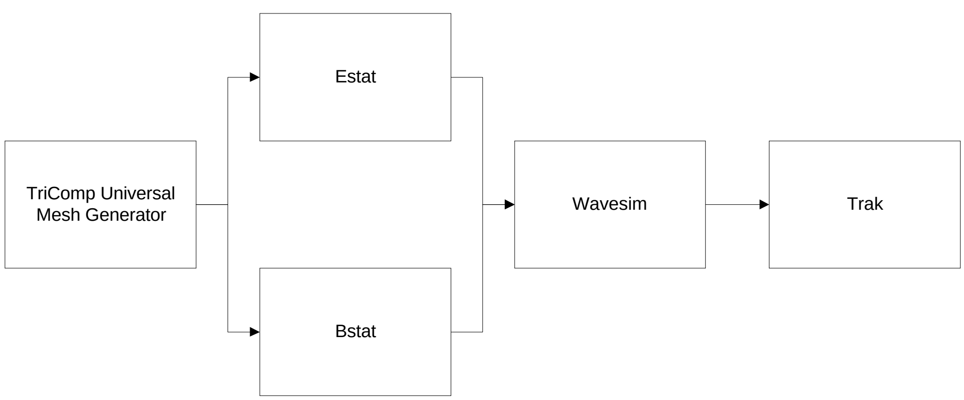

Figure 3. Modeling of Multipacting

Familiarization with the code and multipacting mechanisms will be gained. Typical manufacturing flaws currently observed will be examined by perturbing the surface of the ideal cavity wall geometry. The level of surface perturbations allowed before multipacting becomes serious will be identified. Forced surface perturbations will be identified which will minimize multipacting to compensate for design errors. Presently, the RF cavity ensemble is mechanically compressed or expanded when tuned. Due to slight differences in cavity cell geometry, each cavity cell may not be uniformly compressed. Multipacting as a result of multiple cavities, within the limits of the code, will be examined and compensated for as a result of non-uniformity in structure. Because multipacting is material dependent, materials with different SEC will be examined. A limited number of materials, which can achieve superconducting characteristics in order to minimize wall losses in the cavity, may be available.

Task 2: Computational Fluid Dynamic (CFD) of Niobium Cavities Surface Finish

Surface finish of the niobium cavity plays an important role of achieving the best performance. Even microscopic contaminants on the surface of cavity can seriously affect its performance due to magnetic heating or electron field emission. As a consequence, the surface finish treatment is needed after fabrication of the cavity. Few surface treatment techniques have been widely used. These techniques include chemical etching method, electropolishing method, plasma-spray coating method, high-pressure water peening method, layer particle injection method, rolling and grinding method, honing, and lapping etc. Each method has advantage and disadvantage. For example, electropolishing method can provide a smooth, mirror like surface finish with no sharp steps at the grain boundaries, but the etching rate is slower than chemical etching method. On the other hand, surface contamination by sulfur must be removed by ultrasonic rinsing in hydrogen peroxide in chemical etching. A porous teflon membrane may also needed in cathode to keep the bubbles of hydrogen away from the niobium. Computational fluid dynamics (CFD) simulation is needed to understand the etching process. Computational fluid dynamics techniques are now exerting a tremendous influence on the analysis of fluid flow phenomena, including heat transfer, mass transfer and chemical reaction. We propose using a commercial CFD code for the project, STAR-CD [8]. A symmetric coordinate will be used in 2-D cavity shape design analysis. 3-D numerical simulation will also be studied in case those 2-D numerical results are not satisfied.

The results of this simulation can provide the cavity designer with a way to examine how the chemical solution or coating contacts the walls of the cavity, with or without the flow circulations. Several factors will be considered in the CFD simulation to provide the best surface finish including, different flow rates and flow patterns, i.e. laminar or turbulent flows, with or without agitators or baffles, and temperatures of solution inside cavity.

Task 3: Optimal Design of Niobium Cavities

The first step in the optimizing the niobium cavities is to use a mathematical form for the performance index of the niobium cavities. A measure that is usually used is the quality factor, Q_0 [2], which can be defined as,

$$Q_0 = \frac{\omega_0 U}{P_c}$$

where, U is the stored energy and P_c is the power dissipated in the cavity walls, and ω_0 is the angular frequency of the accelerating mode. The above equation shows minimizing the lost energy and maximizing the stored energy can maximize the quality factor.

The parameters that affect the quality factor include the geometry of the cavity and its surface finish. While spherical cavities yield the best performance with respect to multipacting, elliptical cavities are usually used because of they can be easily manufactured and tuned. They also offer higher mechanical stability. The proposed research include two approaches to create the cavity:

i. Use elliptic geometry
ii. Use spline geometry

In the first approach two variables will be used to describe the cavity, *v* and *c*. In the second approach the cavity will be described using a spline curve. This curve is subdivided into sections, each of them is represented using a spline. Spline curves, expressed in parametric form, use a set of blending functions to combine the effects of *n+1* control points p_i in the form,

$$p(u) = \sum_{\mathrm{i}=0}^{\mathrm{n}} p_i N_{i,k}(u)$$

For B-spline [9] curves, the blending function $N_{i,k}(u)$ the degree of these polynomial is determined using a variable *k*. The blending functions are defined as follows,

$$\begin{aligned} N_{i,k}(u) &= 1 \quad if\ t_i \le u \le t_{i+1} \\ N_{i,k}(u) &= 0 \quad otherwise \end{aligned}$$

and,

$$N_{i,k}(u) = \frac{(u - t_i)N_{i,k-1}(u)}{t_{i+k-1} - t_i} + \frac{(t_{i+k} - u)N_{i+1,k-1}(u)}{t_{i+k} - t_{i+1}}$$

The knot values, t_i, relate the parametric value *u* to the p_i control points. Knot values can be defined as,

$$\begin{aligned} t_i &= 0 && if\ i < k \\ t_i &= i - k + 1 && if\ k \le i < n \\ t_i &= n - k + 1 && f\ i > n \end{aligned}$$

where,

$$\begin{aligned} 0 \le i < n + k \\ 0 \le u < n - k + 2 \end{aligned}$$

Once a performance index is determined, design constraints will be considered. These constraints include geometrical constraints and surface finish constraints. Geometrical constraints ensure that the shape of the cavities is acceptable while the surface finish constraints present the lowest acceptable and the highest possible surface finish quality. Figure 4 summarizes the optimization process for the niobium cavities.

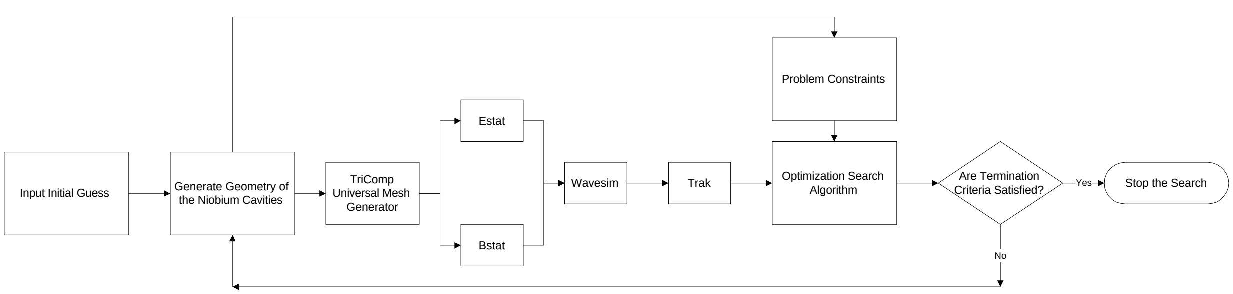

Figure 4. Flowchart for Optimal Design of Niobium Cavities

The problem of maximizing the performance of the niobium cavities will be solved on several stages. The first stage is to determine the appropriate optimization approach by calculating the quality factor for several values of the problem variables. The results will be analyzed, if it is linear or moderately nonlinear, pattern search method will be used. We will start with an algorithm such as Fuzzy Simplex [10], which incorporates fuzzy logic to make the simplex search flexible. Another possible approach is the Twinkling Simplex [11]. In this method a subset of the problem variables are randomly selected for the subsequent simplex movements. If the problem proves to be highly nonlinear, the Successive Heuristic Quadratic Approximation (SHQA) technique [12] will be used. This quasi-random method proved very effective in getting the optimal design for a complex system where the objective function is a result of finite element analysis as in this problem. As familiarity with the problem increases, it may be possible to propose an optimization algorithm that fits with the particulars of this problem.

Capabilities at the University and Los Alamos:

LANL is already active in the area of designing SCRF. Lab personnel collaborated with US industry in the area of cavity fabrication. It is requested that UNLV acquire the necessary software tools for modeling and design of the niobium cavities to enable UNLV researchers to perform work on-campus on this proposal. Additionally, will receive free the research code Trak_RF for our work with LANL, Trak_RF is a research code used to track electron orbits in combined field solutions from EStat, BStat and WaveSim. UNLV will be responsible for the salary and travel of the UNLV researchers while at LANL.

Dr. Schill has been in contact with LANL regarding this project as well as other projects for an extended time. He has been active in research in the area of electromagnetics. Dr. Trabia has worked in optimal design issues. His work in this area has been published in the leading journals and conferences in this area. Dr. Y. Chen brings to this project a unique background of degrees in chemical and mechanical engineering that will be helpful in understanding chemical etching of niobium cavities. Three graduate students would also work on the proposed project.

<u>Equipment Requested for AAA User Labs:</u>

Multipacting: Trak_RF is a research code used to track electron orbits in combined field solutions from EStat, BStat and WaveSim. The following software packages will be purchased from FIELD PRECISION:

i. Trak 5.0 is a well-documented code similar to Trak_RF but does not include the WaveSim component. Trak_RF is a research code and is not well documented. In order to learn to use Trak_RF, we will need Trak 5.0 with documentation.
ii. TDiff is a heat flow code, which may be required to study the thermal impact of multipacting or possible machining.
iii. PAC is a Poisson AC code which should allow us to study the effects of conductive coatings placed over the cavity chamber.
iv. EStat, BStat, and WaveSim are the field codes required to determine the fields in a 2-D axisymmetric geometry.

CFD simulation of chemical etching: The external data interface options in STAR-CD enable the user to exchange data with external CAE software such as CAD systems for some or all of the following functions: surface modeling, mesh generation, and mesh and results display. This important data interface capability will allow the CFD modelers to directly use the CAD geometry meshes from the cavity design team. Different boundary conditions will be then added according to the physical restrictions and domains.

Optimal design of niobium cavities: Matlab is a commonly used tool that allows user to program without the need of recreating low-level mathematical function such as matrix inversion or data plotting. In addition to Matlab, we will be using two of its toolboxes: spline toolbox and optimization toolbox. Spline toolbox is a powerful tool for creating curves and surfaces, while optimization toolbox contains several nonlinear programming subroutines.

Project Timeline:

Timeline Narrative

The proposed research is planned to cover one year, starting in Summer 2001. Research will be conducted with close interaction with appropriate personnel at LANL. We have allocated travel funds for research collaboration with LANL personnel.

The first stage of this project will be dedicated to familiarize researchers and graduate student with various software packages that will be used in this project. In the second stage researchers will integrate the software packages together to optimize the cell design. The last part of the project will be spent in assessing the results. Based on the results at the end of the year, we expect to expand the project by looking at other cell design parameters as well as experimental verification, for a follow-up proposal.

Expected Technical Results:

- A study of multipacting in niobium cavities with multiple cells.
- Investigate the relationship between the shape and surface condition of the cell and its performance.
- Suggestions for improving the results of chemical etching.
- A systematic approach for optimizing the performance of niobium cavities.

Milestones (Based on starting date of May 15th, 2001)

- Modeling of Multipacting: September 2001
- Integrating Field Precision Finite Element Software in Optimization Software: November 2001.
- Creating a CFD model for the chemical etching process: Dec. 2001.
- Deciding suitable optimization technique(s): January 2002
- Suggesting a mechanism for chemical etching: March 2002.
- Preparing final report: May 2002.

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 student participating in this project.

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[11] Mekhilef, M., and M. Trabia, "Successive Twinkling Simplex Search Optimization Algorithms," accepted for presentation at the ASME 27th Design Automation Conference, Pittsburgh, Pennsylvania, September 2001.

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