Modeling, Fabrication, and Optimization of Niobium Cavities: Phase II Final Report

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

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Research Area: Accelerators / Transmuter
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. The second phase has resulted in an experimental setup of a fluid flow experiment with experimentation to be completed in the third year. Some of these results were presented at American Nuclear Society, Student Conference April 2-5, 2003. 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 and presented at the 2003 ANS conference in San Diego.

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 effort 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.

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 impact can lead to the generation of one or more secondary electrons that in turn act as primary electrons. In turn, these electrons may 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). Consequently, RF power is absorbed. It becomes increasingly difficult to increase the RF energy in the cavity as the power supplied to the cavity is increased. 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. In addition, 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.

Figure 1. Schematic Diagram of Niobium Cavities (Executive Summary: Development and Performance of Medium-Beta Superconducting Cavities (LANL))

While models have been suggested for minimizing multipacting [2], a 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 Phase 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. (MESH and WAVESIM) and an optimization program (fuzzy simplex algorithm) within a MATLAB controlling environment. Figure 2 illustrates the end cell geometry of the LANL Beta 64 cavity with its geometric parameters. Eleven parameters describe the geometry. Since evaluating the resonant frequency for all possible geometric combinations of the eleven parameters proved to be a lengthy process, the parameters were tested to determine the sensitivity of the objective function used in the optimization process. The test indicated that the following three variables are of relative significant importance: $r_a$, $\phi_a$ and $\phi_L$. Table 1 lists the fixed parameters of LANL’s APT cavity end cell. The dependent variables and geometric constraints are

\[
x_e = x_{end} + a_e \left(1 - \frac{1}{a_e^2 + \frac{b_e^2}{\tan^2(\phi_L)}}\right)
\]
\[
y_e = y_{end} + b_e \left[1 - \frac{(x_{end} - x_e)^2}{a_e^2}\right]
\]

17.339 cm ≤ $y_a + r_a$ ≤ 29.925 cm

10° ≤ $\phi_a$ ≤ 90°

5° ≤ $\phi_L$ ≤ 20°

3.5 cm ≤ $x_e$ ≤ 14 cm

Initially the three-parameter space was surveyed using a random generator to determine the initial seed geometries satisfying geometrical constraints given by Eq. 1 and Table 1. For each feasible geometrical case found, WAVESIM calculated the pi-mode resonant frequency. In each case, the geometry of the middle cells are left unchanged. The MATLAB controlling program shifts the cells in the y-direction to match the height of the end cell. Three cases were found to fit the geometrical constraint, the resonant frequency criteria and the pi-mode constraint. Table 2 lists the cases found. The three cases were then used as initial seed guesses for the optimization program employing a fuzzy simplex algorithm to generate a design with a target resonant frequency of 700 MHz. As shown in Table 3, case 1 failed to converge. Case 2 and 3 converged to the target frequency within less than 20 iterations. Figures 3 and 4 provide a visual comparison between the initial seed geometry and the optimized geometry. It has been demonstrated that the optimization searches did not converge to the geometry of LANL’s APT cavity. This indicates that there exist alternative cell designs. Although changes in some of these alternative designs may be relatively small, other researchers have shown that small changes may significantly affect the multipacting process. Future multipacting studies will determine if these alternative designs are as robust compared to the existing APT cavity. Figure 5 illustrates the mesh of the LANL APT
cavity. Only two and a half of the five cavities are shown in the figure. The straight section connected to the end cavity is extended far enough that termination effects are negligible.

![Diagram of cavity with labels](image)

**Figure 2** Geometry of the LANL’s APT cavity end cell.

**Table 1.** Fixed Parameters of the End-Cell LANL’s APT Cavity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y_a$ (cm)</td>
<td>16.339</td>
</tr>
<tr>
<td>$L$ (cm)</td>
<td>5.814</td>
</tr>
<tr>
<td>$a_e$ (cm)</td>
<td>2.425</td>
</tr>
<tr>
<td>$b_e$ (cm)</td>
<td>9.700</td>
</tr>
<tr>
<td>$L_o$ (cm)</td>
<td>15.081</td>
</tr>
<tr>
<td>$y_o$ (cm)</td>
<td>8.000</td>
</tr>
</tbody>
</table>

**Table 2.** Details of the best randomly generated end-cell geometries.

<table>
<thead>
<tr>
<th></th>
<th>Case #1</th>
<th>Case #2</th>
<th>Case #3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_a$ (cm)</td>
<td>4.060</td>
<td>4.169</td>
<td>5.022</td>
</tr>
<tr>
<td>$\phi_a$ (rad.)</td>
<td>1.007</td>
<td>1.028</td>
<td>1.114</td>
</tr>
<tr>
<td>$\phi_L$ (rad.)</td>
<td>0.224</td>
<td>0.242</td>
<td>0.194</td>
</tr>
<tr>
<td>Res. Freq. (MHz)</td>
<td>695.91</td>
<td>693.58</td>
<td>671.76</td>
</tr>
</tbody>
</table>
Table 3. Results of optimization search using the best randomly generated geometries given in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>Case #1</th>
<th>Case #2</th>
<th>Case #3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_a$ (cm)</td>
<td>x</td>
<td>4.086</td>
<td>3.985</td>
</tr>
<tr>
<td>$\phi_a$ (rad.)</td>
<td>x</td>
<td>1.019</td>
<td>1.278</td>
</tr>
<tr>
<td>$\phi_L$ (rad.)</td>
<td>x</td>
<td>0.293</td>
<td>0.315</td>
</tr>
<tr>
<td>Res. Freq. (MHz)</td>
<td>Failed</td>
<td>699.16</td>
<td>699.60</td>
</tr>
</tbody>
</table>

Figure 3 Comparison of the random seed end cell (693.58 MHz) to the optimized end cell geometry (699.16 MHz) for Case #2.
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. During this last quarter, an electron gun, heat tape, and a residual gas analyzer (RGA) were received. To save about $55,000 or more, the insides of an old cryogenic pump has been converted to a cryostat. The “cryostat” was tested by the manufacturer and will reach superconducting temperatures for niobium (~8 K). Quotes for a manipulator and load-lock chamber have been obtained. Figure 6 shows the existing cavity with pumps and blanks.

**Figure 4** Comparison of the random seed end cell (671.76 MHz) to the optimized end cell geometry (699.60 MHz) for Case #3.

**Figure 5** Two and a half of the five-cell Beta 64 LANL APT cavity is shown in mesh form.
The choice of sensor is crucial in this experimental study. Both temporal and spatial resolution have to be examined with care assuming an extremely low flux (ones and twos) of secondary electrons are being generated. Two types of sensors are under consideration: low energy electron diffraction (LEED) sensor employing a phosphorous screen and a position sensitive MCP/RAE electron sensor (Vendors: Quantar Technology Inc. or Roent Dek). The latter has a spatial resolution between 50 to 800 µm and can detect single energetic electrons. To determine the resolution required, both a theoretical and a numerical study was performed. The latter is still being refined but initial results are provided here. For a simple back-of-the-envelope calculation, the sensor of radius R₂ and the piece under test of radius R₁ are assumed concentrically oriented, electrically conducting, and hemispherical in shape. (Refer to Figure 7). The z-axis passing through the central portion of the hemispheres exhibiting symmetry in azimuthal angle. The equation of motion for an electron of charge q and mass m launched on the inner sphere on the z axis with potential Vₛ (typically 2 kV to 3 kV) across the two conductors is given by

\[
\begin{align*}
\ddot{r} &= \frac{K₁}{r^2} + \frac{4K₂^2}{r} \\
\dot{\theta} &= 2 \frac{K₂}{r} \\
K₁ &= \frac{qVₛ}{m} \left(\frac{R₁R₂}{R₂ - R₁}\right)
\end{align*}
\]

(2a,b,c)

where K₁ and K₂ are constants of motion and the radius of the niobium sample and the sensor was chosen as R₁=1 cm and R₂=6 cm respectively. Equations 2a and 2b are a consequence of the equation of motion in an electric field neglecting fringe effects. Equation 2c is the nature of the fields between the plates. It is known that the initial energy of a secondary electron ranges between 1 and 20 eV. With this, a range of constants for K₂ can be obtained from the initial energy equation. With the aid of a computer program, worst case spatial deviations from the z-axis on the sensor surface were determined. Table 4 lists some of the extreme deviations from the z-axis for various source voltages, electron energies, and initial electron trajectories. The distance of separation between the sensor and the piece under test was determined by the amount of room in the vacuum cavity. A 5 cm difference is an upper limit in value. The data in Table 4 tends to suggest that the coarsest resolution that may be allowed for meaningful measurements is roughly a millimeter. Spherical sensors do not exist. As a result, computer simulations employing a finite element electrostatic code and a particle
tracking code was used for a more accurate and detailed study of the sensor. Planar rectangular sensors with a centered circular aperture are typical. These computer simulations also exhibit the effects due to the platform supporting the niobium sample, the electron gun and the sensor mount with sensor. Figures 8 and 9 illustrate particle trajectories of 20 eV electrons launched from the sample under test with various initial trajectories. Further studies are being conducted to choose the optimal distance between the sensor and the sample minimizing the size of the sensor. The effect of an intermediate grid is also being studied. These studies are important especially since the sensor size and resolution dictates cost.

**Table 4.** Spatial resolution of sensor is determined by the spatial deviations from the z axis for a range of electron energies and source voltages assuming a maximum 5 cm distance of separation between sensor and piece under test.

<table>
<thead>
<tr>
<th>Initial Energy (eV)</th>
<th>Initial Trajectory</th>
<th>Source Voltage (kV)</th>
<th>Deviation from z axis on sensor surface (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Any energy</td>
<td>Along z axis</td>
<td>Any</td>
<td>0.0</td>
</tr>
<tr>
<td>1</td>
<td>Perpendicular z axis</td>
<td>2</td>
<td>1.2</td>
</tr>
<tr>
<td>1</td>
<td>Perpendicular z axis</td>
<td>3</td>
<td>0.97</td>
</tr>
<tr>
<td>20</td>
<td>Perpendicular z axis</td>
<td>2</td>
<td>5.3</td>
</tr>
<tr>
<td>20</td>
<td>Perpendicular z axis</td>
<td>3</td>
<td>4.3</td>
</tr>
</tbody>
</table>

**Figure 7.** Simple geometry of sensor (outer hemisphere) and niobium piece under test (inner hemisphere).
**Figure 8.** The sample and electron gun are aligned. A 20 eV electron is launched from the surface of the sample under test with various initial trajectories. Electrons exhibiting initial motion normal to or nearly normal to the surface escape through the aperture opening and are not detected. The distance between the sample and the sensor is 5 cm.

**Figure 9.** The sample and electron gun are not aligned. A 20 eV electron is launched from the surface of the sample under test with various initial trajectories. Electrons with different initial trajectories exhibit significant deviations.
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 10. Finite element analysis shows that the baffle partially succeeded in achieving its purpose as can be seen in Figure 11. 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.

![Current Etching Configuration of Niobium Cavities](image)

**Figure 10.** Current Etching Configuration of Niobium Cavities

![Velocity Field for the Current Baffle Design](image)

**Figure 11.** Velocity Field for the Current Baffle Design (inset: zoomed-in view of the flow at the exit)

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 12. 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 12. 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 13. A transparent plexiglass box was manufactured to enclose the cavity. Pump and piping system were also modeled, Figure 14. A complete setup was assembled, Figure 15. The experiment includes a computer-controlled x-y traverse mechanism, Figure 16. The specifications of the traverse are listed in Table 5. The traverse carries a CCD camera, Figure 17. The specifications of the camera are given in Table 6. We developed a program that can activate the traverse to position the camera through a sequence of positions through the workspace.

Figure 13. Photo of the LANL Transparent Cavity
Figure 14. A Model of the Experimental Setup

Figure 15. Experimental Setup
Figure 16. Traverse mechanism and CCD camera

Table 5 Specifications of the Traverse

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Payload</td>
<td>5 lb</td>
</tr>
<tr>
<td>Horizontal Travel (Axis 0)</td>
<td>48 inches</td>
</tr>
<tr>
<td>Vertical Travel (Axis 1)</td>
<td>24 inches</td>
</tr>
<tr>
<td>Straightness</td>
<td>0.0005 in/in</td>
</tr>
<tr>
<td>Positional Accuracy</td>
<td>0.0005 in/in</td>
</tr>
<tr>
<td>Drive Type</td>
<td>Screw</td>
</tr>
<tr>
<td>Motor Type</td>
<td>Stepper</td>
</tr>
<tr>
<td>Controller</td>
<td>Controller should be able to control two motors with RS-232 ports</td>
</tr>
</tbody>
</table>

Revised 6/6/03
First Version
Figure 17. View of the CCD camera

Table 6. Specifications of the Camera

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>2.0” H X 2.7” W X 6.0” L</td>
</tr>
<tr>
<td>Lens</td>
<td>C-Mount</td>
</tr>
<tr>
<td>Weight</td>
<td>1.5 pounds</td>
</tr>
<tr>
<td>Scanning</td>
<td>Non-interlaced, progressive</td>
</tr>
<tr>
<td>Synchronization</td>
<td>Pixel clock internal</td>
</tr>
<tr>
<td>Dynamic Range</td>
<td>48 db 8-bit, &gt;.58 db 10-bit</td>
</tr>
<tr>
<td>Pixel clock rate</td>
<td>20 MHZ</td>
</tr>
<tr>
<td>Frame rate</td>
<td>30 fps in dual channel mode</td>
</tr>
<tr>
<td></td>
<td>15 fps in single channel mode</td>
</tr>
</tbody>
</table>

Dye injection:
The dye is injected in the pipe using a syringe, upstream of the inlet section of the cavity as shown in the Figure 17. The fluid flow pattern, Figure 18, inside the cavity is then recorded as image sequences at regular time intervals using the CCD camera and the imaging software. Knowing the time difference and the displacement of dye between frames, the velocity and corresponding discharge for quantitative analysis are calculated. Using the velocity values at different regions inside the cavity cell the velocity profile for the flow is obtained. A drawback of using dye is that it gets diluted as it moves through the cavity, which makes it difficult to use
for flow visualization away from the point of injection. Figure 19 shows a flow image captured using CCD camera for dye injection.

Figure 18. Dye injection using syringe.

Figure 19. Dye flowing through the cavity.
Figure 20. Flow pattern inside cavity using dye

**Seeding particles:**
Seeding particles are also used as an alternative method to track the flow pattern. Two types of particles are used in the experiment:

1. Silver coated hollow glass sphere is one of the seeding particles used. It is of size 10µm. The silver coating reflects light and renders good visualization, it also has the drawback of settling down as the specific gravity of this particle is greater than that of water.

2. The other seeding particle used is polyamide seeding particles of size 50µm. This is of lower specific gravity and floats in the water. The seeding particles are also injected into the system in a similar fashion as that of dye. Figure 19 shows flow with seeding particles.

Figure 21. Flow pattern using seeding particles
Preliminary conclusion:
The flow visualization results prove that the flow is barely around the baffle structure without much circulation inside the cells, Figure 21. This result is in accordance with the CFD results obtained in the first phase of the project. It is clear that a better baffle design is necessary to improve the flow circulation inside the cells resulting in better etching process.

Figure 22. Flow around baffle

Dissemination of Results
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.” [16]
- Discussions with LANL personnel, especially Dr. Tsuyoshi Tajima
References