

Design and Fabrication of a Custom Scanning Tunnelling Microscope

by

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Abstract

The primary goals of this project are to design and fabricate a custom Scanning Tunnelling Microscope (STM). This STM will be a part of the Ultrafast Microscopy and Magnetism Laboratory and will be used to study sub-picosecond electronic and magnetic dynamics with atomic resolution. The design goals of the STM are to have high vibrational stability, low thermal drift, non-magnetic components in the STM head, and optical access to the tunnelling junction for coupling to THz light. The project has spanned multiple complete design and iterative prototyping cycles for the STM head design initially based on the Pan design [1]. The primary parameters for the STM head design were to minimize mass while preserving rigidity and maximize the first resonant mode frequency. All the components were designed using the Computer-Aided Design software (CAD) Autodesk Inventor and tested for rigidity and resonant modes using Autodesk NASTRAN, a Finite Element Analysis (FEA) software. The tested prototypes were initially 3D printed and then milled out of Aluminum 6061 using Computer Numerical Control (CNC) machines for the final parts.

The final aluminum STM head prototype has been designed, fabricated, and assembled. The lowest calculated resonant frequency of the head is 1.12 kHz. The STM head was tested for coarse motion and failed to produce sufficient displacement. The tests with the aluminum STM head led to a revised design for the 3D-printed titanium STM head and have guided the design methods for future designs that make even more use of 3D printing. The titanium STM head is designed and fabricated and is waiting to be assembled and tested.

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Chapter 1

Background

1.1 Introduction

In 1959, Richard Feynman gave a speech titled “There’s Plenty of Room at the Bottom” to the American Physical Society, inviting physicists to develop a new technology to image and manipulate individual atoms [2, 3]. Feynman theorized that such devices would contribute to the denser computer circuitry and provide a better understanding of the fundamental problems in molecular biology [4]. The two main microscopes available at that time were optical and electron microscopes. Optical microscopes had a hard resolution limit set by the wavelength of the light used and diffraction [5]. Electron microscopes, on the other hand, have a much higher resolution, but the technology to build electron optics of high quality was limited at that time. Therefore, Feynman’s challenge was not met until the inventions of the Scanning Tunnelling Microscope (STM) and the Atomic Force Microscope (AFM) [6].

The Scanning Tunnelling Microscope (STM) was one of the first instruments that allowed the direct imaging of atoms. The invention of the STM by the physicists Gerd Binnig and Heinrich Rohrer [7, 8, 9] led to them winning the 1986 Nobel Prize in Physics. An STM fundamentally differs from optical and electron microscopes due to its non-reliance on wave or particle diffraction for imaging. The STM scans samples using an atomically sharpened tip that is brought extremely close ($> 1\text{nm}$) to the sample’s

surface with a bias voltage applied. This voltage allows electrons to tunnel between the sample and the tip (or vice versa), forming a tunnelling current. The measurement of this tunnelling current allows for the precise calculation of the distance between the sample and the tip. As the tip moves along the surface of the sample, a topographical map of the surface can be made with atomic resolution. However, this technique limits the STM to only image conductive materials, superconductors, semi-insulating surfaces and semiconductors.

In the decade after the invention of the STM, monumental advancements were made in the fields of nanotechnology and nanoscience. This, in turn, helped STMs progress rapidly in the late '80s and early '90s and led to some groundbreaking experiments such as the surface conductivity mapping and later the mapping of magnetic domain structures using a modified version of the STM called the spin-polarised STM (SP-STM). The STM has continued to evolve since then, with its flexibility allowing it to be used in various fields of science. Some of the modern capabilities of the STM are its capability to manipulate atoms [10], ultrafast time resolution [11], and inelastic transfer of energy from a tunnelling electron to excite molecular vibrations [12] or spins [13].

The flexibility of the STM, along with its ability to be spin polarised and have ultrafast time resolution, makes it the ideal apparatus to image magnetic dynamics at the atomic scale. Some of the more recent developments also support this statement, such as the ability to map exact electron band structure in momentum space by Fourier transforming images of surface state [14], improved time-resolved techniques allowing measurements of spin relaxation [15] and sub-picosecond time resolution [16]. The STM is also a very versatile equipment that will play a significant role in condensed matter physics, chemistry and nanotechnology in the future. With every new application of the STM, we discover more capabilities of this apparatus, such as its ability to study many phenomena from micro to nanometer scale, including the strength of chemical bonds, dielectric properties, contact charging, molecular manipulation, local electronic states, artificial atomic structures, single defects and many more. Therefore, the construction of an STM at the University of Manitoba will not only allow us to image magnetic dynamics at the atomic scale but also help various other research projects happening at the university by providing a different and more unique way to study samples at the

atomic scale.

1.2 Introduction to Scanning Tunnelling Microscopes

Scanning tunnelling microscopes are instruments used to make topographical maps of samples' surfaces at atomic scales (as discussed in the earlier sections). Here, we go into more detail on how an STM functions, as well as its other capabilities, which makes it an ideal instrument for condensed matter physicists to study material properties.

1.2.1 STM Operation

The primary part of an STM that does all the scanning is the STM head. The typical STM head consists of four main components: the coarse z-motor, the tube scanner, the probe tip and the sample holder. The tube scanner is a cylindrical tube made of piezoelectric ceramic with a metal coating that acts as electrodes. The z-motor uses shear plate piezoelectric stacks held in tension to provide coarse motion in the z-direction. Piezoelectric ceramics are materials that can provide mechanical motion or deformation when there is a voltage difference applied across them. Since the deformations are extremely small and accurately reproducible, they make the ideal scanning probes and motors when nanoscopic movements are needed.

This abundant use of piezoelectric materials in the STM head for all motions makes it the heart of the design, and without the precise motion provided by the piezoelectric tube scanner an STM would not exist.

The way an STM tip scans a sample is by initially having the sample set up a few millimetres from the tip and using the coarse motor to move the head closer using shear plate piezos. The primary role of the coarse motor is to bring the STM tip about 50-100 nanometers away from the sample's surface. The coarse motor usually determines the quality of the STM since the tube scanner that does all the fine movements is ubiquitous. The design, fabrication, and material choices set the performance and the rigidity of the STM, and most of the advances in STM are based around coarse motor design and

upgrades. The modern design for the coarse motor is the Pan design [7], and the most advanced STMs of today are upgraded versions of it. In this design, coarse motion is made using stacks of piezoelectric shear plates. Once the coarse motor moves the head and is in position for scanning, the tube scanner takes over for all fine motions. All scanning is done with the probe tip extremely close to the sample ($> 1\text{nm}$) but not physically touching the sample. When the STM is ready for scanning, a bias voltage is applied to the sample, favouring a flow of electrons between the sample and the probe tip. Since the probe tip and the sample are never physically in contact with each other, the flow of electrons is only possible through the phenomenon of quantum tunnelling. Therefore, this flow of electrons is called the tunnelling current. The probability of an electron tunnelling through this gap is influenced by the overlap of the electron wave functions, which extend beyond the surfaces of the probe tip and the sample into the vacuum gap in between them. The overlap of the two wavefunctions, in general, depends exponentially on the distance between the sample and the probe tip. This means that the tunnelling current is a good indication of the width of the tunnelling gap.

The most common way to make a topographical map of a sample's surface is to do a raster scan while using a feedback loop to hold the tunnelling current constant. This maintains a constant gap between the sample and the tip as the tip moves along the sample's surface. The surface is imaged by measuring the extensions and contractions of the scan tube as it moves the tip along the sample's surface. This mode of operation is called the constant current mode, as the tunnelling current is the fixed parameter. The second mode of scanning is the constant height mode. Here, the tube scanner is fixed, and the change in tunnelling current as the tip moves over the sample's surface is recorded. Since height is constant, this mode of operation is riskier for tip crashes. As the height of the tip is fixed, if the topography of the sample has a broad range, there could be a point where the tip and the sample could come into contact and damage the sharpness of the tip. This makes the constant height scanning mode less popular.

The topographical information gained from an STM is only approximate, as other factors affect the tunnelling current between the tip and the sample. One of the more interesting properties that affect the tunnelling current is the electronic density of states over the sample's surface. This variation reveals excellent details about the

sample's electronic structure and can be isolated by the third mode of scanning tunnelling microscopy called Scanning tunnelling spectroscopy (STP). In this mode, the tip is fixed over a point on the sample's surface, and the bias voltage applied to the sample is changed to obtain spectroscopic data. This can be done at a single point on the surface of the sample or at a grid of points covering the area of the sample surface.

1.2.2 Types of STM

In addition to the standard STM, this project makes use of some other subtypes as well. The first type is the conventional STM, which makes topographical maps of the sample's surfaces, as explained in the previous section. The second type is the Spin Polarised STM (SP-STM), and the third is the THz-coupled STM. These three types of STMs can also be classified as the evolution of the STM over the years, increasing its capabilities. However, since the functions of these three STMs are quite different, they can be treated as three types of STM for this instance.

The primary difference between a conventional STM and a SP-STM is the probe tip. In an SP-STM, the electrons in the probe tip have the same spin orientation. As the tip scans over the surface of the sample, the electrons with a similar spin to that of the tip will have a higher chance of tunnelling through the vacuum gap between the tip and the sample. This phenomenon allows the SP-STM to image the magnetic properties of the sample's surface, such as the spin and domain walls.

A THz-coupled STM uses THz light pulses to induce electron tunnelling through the gap between the sample and tip instead of using a bias voltage. This allows the STM to achieve temporal resolution, allowing the imaging of dynamics on samples at atomic scales. The time resolution is achieved using the stroboscopic (pump-probe) technique.

1.2.3 Vacuum

STMs can operate in the atmosphere or even submerged in a liquid. However, the gas molecules in the tunnelling junction can easily interfere with the tunnelling current by

interacting with the tunnelling electrons. These gas molecules can also interact with the surface of the sample and introduce contaminants that could affect the scan results. For this project the STM requires an ultra-high vacuum (UHV) chamber to achieve the resolution targeted. UHV conditions allow clean surfaces to be prepared and provide low background noise. We are also interested in cryogenic measurements, which is ideal in UHV environments as any molecules that are present in the tunnelling junction will have much less kinetic energy to interfere with the scans.

This can be further illustrated by a simple calculation of the gas flux in the atmosphere, assuming the STM is in a 1 cubic meter chamber.

The equation for gas flux is

$$\Phi = \frac{1}{4} \frac{N}{V} \sqrt{\frac{8kT}{\pi m}} \quad (1.1)$$

where,

$$\begin{aligned} \frac{N}{V} &= \text{number density of the molecules} \\ T &= \text{temperature} \\ k &= \text{Boltzmann constant} \\ m &= \text{mass} \end{aligned} \quad (1.2)$$

Assuming the gas is pure nitrogen, and the chamber is at 300K, we have

$$\Phi = 8.66 \times 10^{27} \text{ collisions/m}^2 \text{ s} \quad (1.3)$$

Therefore, the number of molecules interacting with a 1nm² area is

$$\Phi = 8.66 \times 10^9 \text{ collisions/nm}^2 \text{ s} \quad (1.4)$$

The gas flux in a UHV chamber at 300K can be calculated the same way as well.

$$\begin{aligned}\Phi_{UHV} &= 2.93 \times 10^8 \text{ collisions/m}^2 \text{ s} \\ \Phi_{UHV} &= 0.29 \text{ collisions/nm}^2 \text{ s}\end{aligned}\tag{1.5}$$

At cryogenic temperatures ($\sim 10\text{K}$), the gas flux drops down to

$$\Phi_{UHV} = 0.05 \text{ collisions/nm}^2 \text{ s}\tag{1.6}$$

This gives us a basic understanding of how much noise a room-temperature STM exposed to the atmosphere will have in its scans compared to an STM at UHV and cryogenic temperatures.

1.3 Motivation

The primary goal of this project is to make an instrument that is capable of imaging magnetic dynamics at the atomic scales. The instrument chosen (STM) is used in various fields, from nanotechnology to chemistry and biology [17]. Studying and understanding magnetic dynamics such as spin waves and domain walls will help many fields, from semiconductor technology to medical fields [18]. One of the areas of particular interest to this project's future work is spintronics.

1.3.1 Magnetism

Magnetic properties of materials arise from the spin and the orbital motion of the materials' electrons [19]. All materials can be divided into two groups by their magnetic properties: materials with permanent magnetic moments and those without. Materials with permanent magnetic moments can be further divided into two groups depending on their manifestation of the long-range ordering of the magnetic moments. Lastly, materials with magnetic order are classified according to their magnetic moments' particular alignment pattern, as shown in Figure 1.1 [20].

Magnetic properties can also be explained using magnetic susceptibility $\bar{\chi}$ by the following equation

$$\mathbf{M} = \mathbf{M}_0 + \bar{\chi} \cdot \mathbf{H} \quad (1.7)$$

where $\mathbf{M}$ is the net magnetic moment per unit volume (magnetization), $\mathbf{H}$ is the applied field, and $\mathbf{M}_0$ is the spontaneous magnetization without an applied field. Usually, $\bar{\chi}$ is represented by a 3×3 matrix.

All magnetic properties of materials are an effect of the spin angular momentum of its electrons.

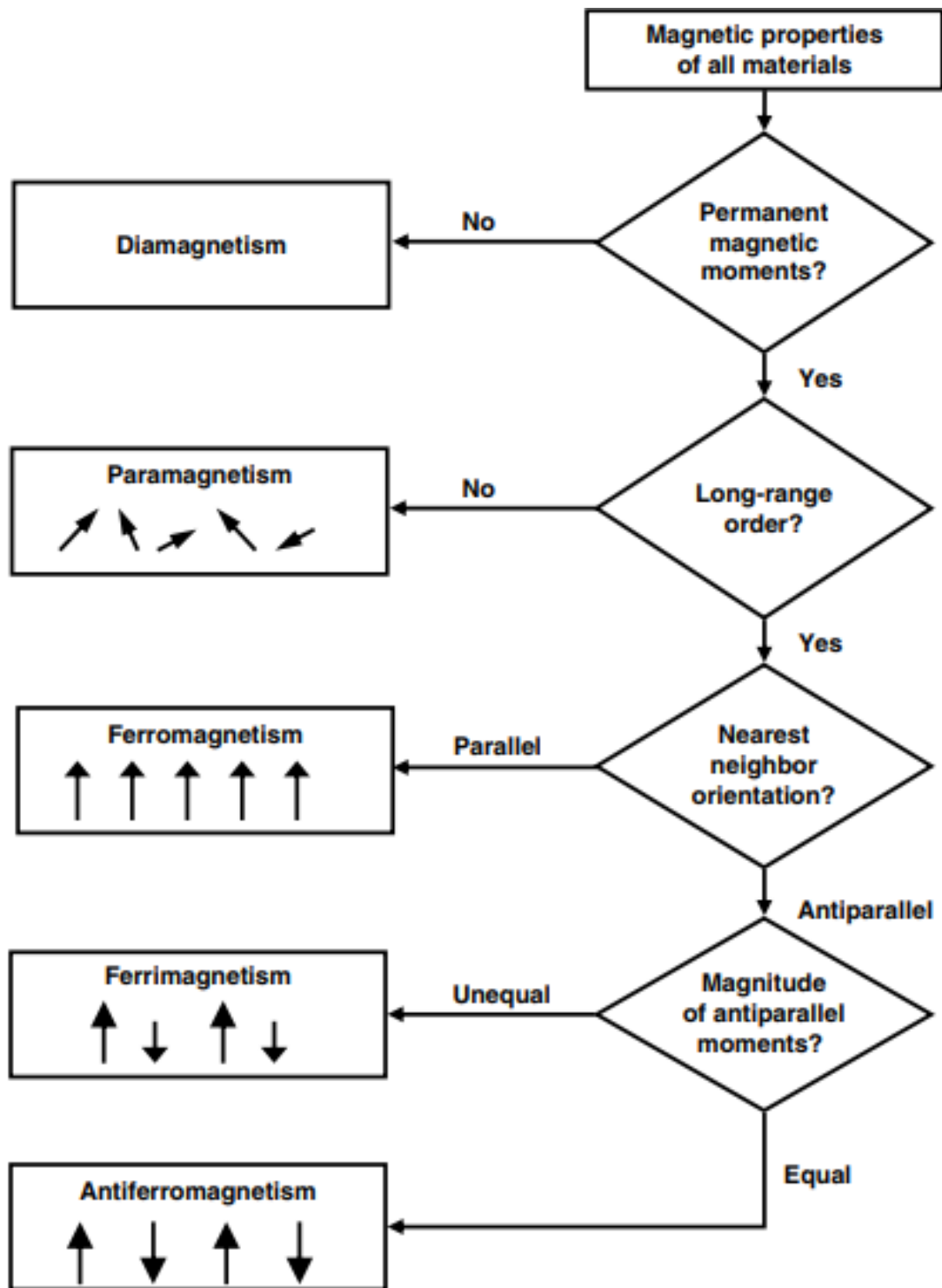


Figure 1.1: Classification of materials according to their magnetic properties [20].

1.3.2 Spintronics

In the middle of the 20th century, it was discovered that spin plays a fundamental role in magnetism. By the late 20th century, digital information was gaining importance, and it was realized that spin could be harnessed to process this information encoded with binary bits of 0 and 1. This is the primary theme of spintronics today [21], [22]. Spintronics also deals with more traditional areas of magneto-electrodynamics, such as magneto-resistive effects for sensing and storing information. Some of the early successful inventions that came out of spintronics are non-volatile magnetic random-access memory (MRAM) [23], read heads for magnetic storage media, programmable spintronic logic devices [24], rotational speed control systems [25], positioning control devices [26], devices for power systems [27], etc.

Spintronics' ultimate goal is to replace semiconductor-based computing technology. Conventional semiconductor devices use the movements of electrons (current) to control transistors, which is an energetically expensive process. As technology advances and the need for more compact and efficient devices rises, the size of the transistors is miniaturized to meet this demand. However, this temporary solution reaches a limit as the transistor sizes reach atomic scales. Even the current efficiency and optimization gains cannot keep up as the global demand for power from computing devices continues to grow [28]. As the world switches over to an information-based economy and the requirement and reliance on technology rises, the strain on the global energy supply could slow growth. A new, more efficient kind of computational device is needed to overcome this obstacle, and spintronics hopes to be the solution.

The primary difference between spintronic devices and conventional semiconductor based devices is that semiconductors primarily use electrons' movement for their functions. In contrast, spintronic devices use the dynamic manipulation of the direction of magnetic moments in magnetic materials to function [29]. Encoding information in the magnetization of materials offers various advantages, such as non-volatile memory (memory devices do not require power to store data), and the energy required to reorient the magnetic moments is far less than that is used to confine charges in semiconductor devices. Modern spintronic devices can be built on decades of research and development

for magnetic hard drives and push beyond their relatively slow read and write speeds. This technological advancement could be achieved by finding better ways to manipulate the magnetic moments of materials. The current understanding of magnetic dynamics needs to be improved for this, and one of the fundamental steps for that is to image and observe magnetic dynamics with unprecedented detail.

1.3.3 Ultra-fast Time Resolved Spin-polarised STM

Spin waves and magnons have been studied by physicists for decades now. However, there hasn't been an instrument that has the capability to image magnons with time resolution and is sensitive to atomic resolution, and this project aims to set up the groundwork for such an instrument.

A Scanning Tunnelling Microscope is the ideal instrument to provide the detail required to study magnetic dynamics at atomic scales. As discussed before, a conventional STM can only make topographical maps of the surfaces of sample and to study magnetic properties a SP-STM needs to be used. However, SP-STMs can only be used to make static images of the spin orientation on the surface of the sample, and they provide no time resolution. They are also very slow when it comes to scanning, which is why they are usually used for samples that are in equilibrium. These slow scans are suitable for studying magnets with dynamic properties that span geological timescales, such as permanent magnets. Still, we need a new kind of STM to study magnetic dynamics at sub-picosecond timescales.

Faster time resolution can be achieved by using optical techniques known as pump-probe experiments [11]. Combining the pump-probe method with an SP-STM and a THz-coupled STM could lead to the Ultra-fast THz-coupled SP-STM, which will have the time resolution required to image individual spin precession. The bias voltage will be replaced with THz pulses to induce tunnelling in this particular instrument. The slow STM electronics will measure the averaged current over millions of THz pulses, and the ultrafast information must then be separated from it. In this experiment, the sample will be perturbed before being scanned with an infrared pulse that precedes every THz pulse that is used for scanning. This process allows the STM to measure the transient process

after the sample is disturbed. The time delay between the infrared and THz pulses can be controlled using standard optical delay lines. By measuring the relationship between the change in time delay and the tunnelling current, the response to the stimulus by the infrared pulse can be extracted. This pump-probe technique allows STMs to make ultrafast measurements [16].

An STM that combines spin polarization with ultrafast time resolution would be able to study magnetodynamics at atomic scales. With the unprecedented resolution in magnetodynamics provided by this STM, we could gain a better understanding of how to build the next generation of computers. This project works towards this goal by developing key components of such an instrument.

1.4 Outline

The objective of this master's project is to design and fabricate a custom STM that is capable of imaging magnetic dynamics at the atomic scales. For this, the STM head must be ultra-high vacuum compatible, should minimize the impact of vibrational modes (high resonance frequencies), be built out of non-magnetic materials, have low thermal drift and allow access to pulses of THz light to the tunnelling junction. In this thesis, the design, fabrication of the STM head and the design analysis are presented. Significant challenges to the STM design are also discussed, and new and alternate ways of fabrication for the next prototype are presented. A custom STM reduces the cost significantly and fits into all the constraints required for future experiments in the ultrafast microscopy and magnetism laboratory compared to pre-built solutions. Another advantage of the custom STM is the ability to upgrade it over time and add modifications as needed without voiding any warranties like with pre-built STMs.

The primary theory required for the understanding of the STM functionality is provided in Chapter 2, including the theory behind the piezoelectric motors used in the STM head. Chapter 3 explains the design choices and the procedure followed for the Finite Element Analysis (FEA). In Chapter 4, the fabrication processes used in the current prototype of the STM head, and its limitations are discussed. There is also a

subsection here that describes the additive manufacturing capability that we received at the last stages of this project.

Chapter 5 focuses on the assembly of the STM head and the ultra-high vacuum (UHV) chambers. Wiring of the STM is a significant focus of this chapter as well due to the problems that were faced during this process. In Chapter 6, the next prototype of the STM that was fabricated using additive manufacturing processes is discussed, as well as the advantages and the possibilities this process brings to the table in terms of the material choices as well as dimensional accuracy. Additive manufacturing is still in its early stages when it comes to usage in UHV environments, so additional compatibility tests had to be done to test the capabilities of the 3D-printed parts.

Chapter 7 brings all the previous chapters together and discusses the results and challenges of all the other chapters.

Chapter 2

Scanning Tunnelling Microscopy

The scanning tunnelling microscope converges various physics fields and owes its existence to two pivotal phenomena: quantum tunnelling and piezoelectricity. This chapter will delve into the fundamental theory necessary for understanding the physics behind the operation of an STM.

2.1 Theory

Most solids are bonded by the attractive electrostatic interaction between electrons and the nuclei [30]. Many properties of matter depend on the behaviour of valence electrons involved in bonding atoms together in crystals. Two main types of bonds create crystals: ionic bonds and covalent bonds. Ionic crystals are a result of electrostatic interaction between oppositely charged ions. Covalent bonds are usually formed by two electrons partly localized between the atoms they are from, and the spins of these two electrons are antiparallel. However, a broad spectrum of crystals exists between the ionic and covalent limits.

A crystal with a large number of free electrons that are available to move within is classified as a metal. These abundant free electrons make metals good conductors, and the binding energy of metal crystals is much less than other crystals. For the STM, a metallic tip-to-sample junction is used because of the free motion of electrons. STMs

can also scan with semiconductor–insulator–semiconductor and semiconductor–insulator–metal tunnelling junctions. Quantum tunnelling is a classically forbidden phenomenon where a particle moves through a potential barrier.

The behaviour of the free electrons in metal at a tunnelling junction of two conductors can be studied by modelling the electrons as free particles in a box.

2.1.1 Density of States

The density of states (DOS) describes the number of allowed modes per unit energy range for electrons. One can look at the free electron gas model to understand the density of states in three dimensions. Here, we start with the free-particle Schrödinger’s equation [30].

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}). \quad (2.1)$$

Assuming the free electron gas is confined to a cube of length L , the solution to the wavefunction simplifies to

$$\psi_n(\mathbf{r}) = A \sin\left(\frac{\pi n_x x}{L}\right) \sin\left(\frac{\pi n_y y}{L}\right) \sin\left(\frac{\pi n_z z}{L}\right), \quad (2.2)$$

where n_x , n_y and n_z are positive integers.

Here, we can assume that the crystal is infinite, allowing us to ignore the effects of the outer boundaries of the crystal. And require that our wave function be periodic in x , y and z directions such that

$$\psi(\mathbf{x} + \mathbf{L}, \mathbf{y}, \mathbf{z}) = \psi(\mathbf{x}, \mathbf{y}, \mathbf{z}). \quad (2.3)$$

The wavefunction that satisfies these boundary conditions and is the solution to Schrödinger’s equation has the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = Ae^{(i\mathbf{k}\cdot\mathbf{r})}, \quad (2.4)$$

given that k satisfy

$$k_x = \frac{2\pi n_x}{L}; \quad k_y = \frac{2\pi n_y}{L}; \quad k_z = \frac{2\pi n_z}{L}. \quad (2.5)$$

Substituting this into the Schrödinger equation gives us the energy of the orbital with wavevector as

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2). \quad (2.6)$$

A sphere can be used to represent the occupied orbitals in k space. When a system has N free electrons in the ground state, the surface of the sphere is called the Fermi surface. Fermi surface shape and volume determine the electrical properties of the metal as current is produced by the change in the occupancy of states at the Fermi surface. The energy at the topmost level is called the Fermi energy; in this case, that will be the surface of the sphere. Wavevectors at the Fermi energy level are called the Fermi wavevectors and are represented by the following equation.

$$k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3} \quad (2.7)$$

where N is the number of electrons, and V is the volume in k space. From here, we can derive the expression for the number of orbitals per unit energy range, which is the density of states for the system [30]. This derivation is for a free electron gas.

$$D(\epsilon) \equiv \frac{dN}{d\epsilon} = \frac{V}{2\pi^2} \cdot \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot \epsilon^{1/2} \quad (2.8)$$

This density of states defines the number of electrons occupying a given energy state. In an STM, tunnelling depends on the density of states of the tip and the sample. Effectively, a net tunnel current can arise when electrons occupying states on one side of

the junction can reach unoccupied states on the other without gaining or losing energy (to first order). The more interesting densities of states can be studied using the STM made for this project, such as spin-split DOS, topological insulators, semiconductors, high-temperature superconductors, etc.

2.1.2 Tunnelling Phenomenon for STMs

Tunnelling is the phenomenon of the propagation of particles through a potential barrier. This is a fundamental feature distinguishing quantum mechanics from classical mechanics. In a classical case, when a particle reaches a potential barrier where its kinetic energy would be negative, it will either bounce back or halt. In the quantum case, the particle has wave-like properties and can tunnel through the barrier. The STM mostly relies on the metal-insulator-metal tunnelling junctions, which is an extensively studied topic [4]. Multiple theories describe these systems, but the pre-eminent quantitative theory used for STMs is Bardeen's first-order perturbation theory, developed in the '60s. This theory was initially developed to understand the tunnelling junctions between thin films of conductors separated by a very thin insulating barrier and later modified to describe STM tip tunnelling junction by Tersoff and Hamann [31], as well as Chen [32], [33]. Bardeen's theory works best when the tip and sample are sufficiently apart and the bias voltage is low enough [34].

A basic interpretation of quantum tunnelling is shown in Figure 2.1. Here, the tunnelling junction is between a conductive sample and the STM tip, and the barrier is a length of s . The vacuum barrier between the two conductors has an exponentially decaying wavefunction, while the conductive regions have sine wavefunctions for the electron. Here, the exponentially decaying wavefunction results in a non-zero chance of an electron existing at $z > s$. If, in addition, the sample or the tip is held at a potential V with respect to each other, it will be energetically favourable for electrons to transition to the positively charged side, and there will be a flow of electrons called the tunnelling current.

Bardeen's Theory of Tunnelling: One-Dimensional Case

Bardeen's tunnelling theory can be extended to explain non-planar tip-vacuum-sample geometry. There are two approaches to Bardeen's theory: non-equilibrium Green functions and the traditional approach. The conventional approach is discussed here. Some of the assumptions made for the original derivation are [35]:

- The two sets of wavefunctions are approximated to be orthogonal.
- Electron tunnelling is treated as a single particle event (mutual interaction is neglected).
- Both the sample and the tip are in electrochemical equilibrium (both electrodes have the same Fermi energy).
- Direct interactions between the tip and the sample forming coupled electronic states are also neglected. This is only valid if the tip and sample are sufficiently far away ($\cong 4 \text{ \AA}$) [4].

Chen [4] derives the form of Bardeen's solution for the tunnelling current by initially assuming the electrodes to be far away and treating the electrodes as independent systems. Since electron-electron interactions are neglected, we can assume that the electrons are independently governed by the single-electron Hamiltonian:

$$H\psi = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) \quad (2.9)$$

Here, $V(\mathbf{r})$ is the electrostatic potential energy of an electron at position $\mathbf{r}$. Then, the electron dynamics can be solved using the analysis of the single electron Hamiltonian. Since the tip and the sample are assumed to be far away initially, they can be treated as independent systems to estimate the current through the tip-sample junction. Therefore, the Hamiltonians become,

$$H_{\text{sam}} \psi = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + V_{\text{sam}}(\mathbf{r})\psi(\mathbf{r}), \quad (2.10)$$

$$H_{\text{tip}} \phi = -\frac{\hbar^2}{2m} \Delta \phi(\mathbf{r}) + V_{\text{tip}}(\mathbf{r}) \phi(\mathbf{r}). \quad (2.11)$$

Here, the space is divided into three regions: the tip, barrier, and sample regions. The Hamiltonian in the barrier takes a similar form. V_{tip} and V_{sam} are the potentials at the tip and the sample regions, respectively. The eigenfunctions of the tip and sample Hamiltonians are called tip states and sample states, respectively. In this case, the transfer of electrons from the tip states to the sample states (or vice versa) under the influence of the Hamiltonian 2.9 is called the tunnelling current. One of the primary assumptions made here is that the density of states of the tip and the sample are fixed and do not change with the flow of electrons.

Now, looking at an electron in the sample state ψ with energy $\mathcal{E}$, so that

$$H_{\text{sam}} \psi = \mathcal{E} \psi. \quad (2.12)$$

Then, using the Hamiltonian 2.10 for the sample state, we can write

$$\psi(t) = e^{-it\mathcal{E}/\hbar} \psi + \sum_k a_k(t) \phi_k. \quad (2.13)$$

Where $\sum_k a_k(t) \phi_k$ is the sum over all the bound states in the tip such that $H_{\text{tip}} \phi_k = E_k \phi_k$.

Now, we want to find the coefficients of $a_k(t)$. We know that $a_k(0) = 0$ for all k . Then, using the time-dependent Schrödinger equation for the STM, we get:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) &= H \psi(\mathbf{r}, t) = H(e^{-it\mathcal{E}/\hbar} \psi) + \sum_k a_k(t) H \phi_k \\ &= e^{-it\mathcal{E}/\hbar} (H_{\text{sam}} + (H - H_{\text{sam}})) \psi \\ &\quad + \sum_k a_k(t) (H_{\text{tip}} + (H - H_{\text{tip}})) \phi_k \\ &= e^{-it\mathcal{E}/\hbar} \mathcal{E} \psi + e^{-it\mathcal{E}/\hbar} (H - H_{\text{sam}}) \psi \\ &\quad + \sum_k a_k(t) (E_k \phi_k + (H - H_{\text{tip}}) \phi_k) \end{aligned} \quad (2.14)$$

We can also differentiate equation 2.13 to get:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \mathcal{E} e^{-it\mathcal{E}/\hbar} \psi + i\hbar \sum_k \frac{d}{dt} a_k(t) \phi_k \quad (2.15)$$

Therefore, equating 2.14 and 2.15 gives the following after $\mathcal{E} e^{-it\mathcal{E}/\hbar} \psi$ is cancelled from both sides.

$$i\hbar \sum_k \frac{d}{dt} a_k(t) \phi_k = e^{-it\mathcal{E}/\hbar} (H - H_{\text{sam}}) \psi \sum_k a_k(t) (E_k \phi_k + (H - H_{\text{tip}}) \phi_k) \quad (2.16)$$

Taking the inner product of both sides with ϕ_j , we get

$$i\hbar \frac{d}{dt} a_j(t) = e^{-it\mathcal{E}/\hbar} \langle \phi_j | H - H_{\text{sam}} | \psi \rangle + E_j a_j(t) + \sum_k a_k(t) \langle \phi_j | H - H_{\text{tip}} | \phi_k \rangle. \quad (2.17)$$

Here, we assume tunnelling is weak enough so that only the first-order approximations are valid. Therefore, $a_k(t) = 0$ for, which gives us

$$i\hbar \frac{d}{dt} a_j(t) = e^{-it\mathcal{E}/\hbar} \langle \phi_j | H - H_{\text{sam}} | \psi \rangle + E_j a_j(t). \quad (2.18)$$

We know that $a_j(t) = 0$ at $t = 0$, then the solution becomes

$$a_j(t) = \frac{e^{-it\mathcal{E}/\hbar} - e^{-itE_j/\hbar}}{\mathcal{E} - E_j} \langle \phi_j | H - H_{\text{sam}} | \psi \rangle. \quad (2.19)$$

Therefore,

$$|a_j(t)|^2 = \frac{4 \sin^2(t(E_j - \mathcal{E})/2\hbar)}{(E_j - \mathcal{E})^2} \left| \langle \phi_j | H - H_{\text{sam}} | \psi \rangle \right|^2. \quad (2.20)$$

The transition probability of electrons is $|\langle \phi_j | \psi(t) \rangle|^2$. So, we can relate 2.20 to the transition probability using equation 2.9 and get

$$\langle \phi_j | \psi(t) \rangle = a_j(t) + \langle \phi_j | \psi \rangle e^{-it\mathcal{E}/\hbar}. \quad (2.21)$$

Therefore, the approximate rate at which electrons transfer from the sample state ψ to the tip state is $\frac{d}{dt} \sum_j |a_j(t)|^2$, if $\langle \phi_j | \psi \rangle$ is small compared to $a_j(t)$.

$$|\langle \phi_j | \psi(t) \rangle|^2 \cong |a_j(t)|^2. \quad (2.22)$$

So the total rate of scattering of an electron in sample state ψ to a given tip state is,

$$\frac{d}{dt} \sum_k |a_k(t)|^2 = \frac{d}{dt} 4 \sum_k \frac{\sin^2(t(E_k - \mathcal{E})/2\hbar)}{(E_k - \mathcal{E})^2} \times |\langle \phi_k | H - H_{\text{sam}} | \psi \rangle|^2. \quad (2.23)$$

The summation in equation 2.23 can be approximated using Fermi's golden rule as there are many tip states [34]. Although each STM tip is different, the density of states is nearly constant on the energy levels of 10 meV [34]. Therefore, the Fermi golden rule can be applied here.

An application of Fermi's golden rule for this case is to approximate the sum in equation 2.23 by an integral with respect to energy. The right-hand side of the equation can be simplified to

$$\sum_k P_t(E_k - \mathcal{E}) \mathcal{M}^2(\phi_k, \psi), \quad (2.24)$$

where $\mathcal{M}^2(\phi_k, \psi) = |\langle \phi_k | H - H_{\text{sam}} | \psi \rangle|^2$ and $P_t(x) = \sin^2(tx/2\hbar)/x^2$. If we let $N_{\mathcal{E}}$ be the number of tip states with the energies in the interval $-2\hbar/t + \mathcal{E} < \epsilon < 2\hbar/t + \mathcal{E}$ and set

$$\mathcal{M}^2(\psi) = \frac{1}{N_{\mathcal{E}}} \sum_{k: |E_k - \mathcal{E}| < 2\hbar/t} \mathcal{M}^2(\phi_k, \psi). \quad (2.25)$$

Equation 2.24 can be approximated as

$$\sum_k P_t(E_k - \mathcal{E}) \mathcal{M}^2(\phi_k, \psi) = \mathcal{M}^2(\psi) \rho_{\text{tip}}(\mathcal{E}) \frac{\pi t}{2\hbar}. \quad (2.26)$$

Since,

$$\begin{aligned} \int_{-2\hbar/t}^{2\hbar/t} P_t(E) dE &\cong \frac{\pi t}{2\hbar} \\ \sum_k P_t(\mathcal{E}) &\cong \rho_{\text{tip}}(\mathcal{E}), \end{aligned} \quad (2.27)$$

substituting 2.26 into the right hand side of 2.23, we get

$$\frac{d}{dt} \sum_k |a_k(t)|^2 \approx \frac{d}{dt} \left(\frac{2\pi t}{\hbar} \mathcal{M}^2(\psi) \rho_{\text{tip}}(\mathcal{E}) \right) = \frac{2\pi}{\hbar} \mathcal{M}^2(\psi) \rho_{\text{tip}}(\mathcal{E}). \quad (2.28)$$

Equation 2.28 is the rate of electron transfers between a the sample state ψ and the tip states with similar energy, assuming the tip states are vacant. However, the Pauli exclusion principle states that only one electron can occupy a given state. Therefore the density of states $\rho_{\text{tip}}(\mathcal{E})$ must be multiplied by the fraction of the unoccupied tip states with energy $\mathcal{E}$. Therefore the rate of electron transfers from ψ into a tip state becomes

$$\frac{d}{dt} \sum_k |a_k(t)|^2 = (1 - F_{\mu_t, \theta}(\mathcal{E})) \frac{2\pi}{\hbar} \rho_{\text{tip}}(\mathcal{E}) \mathcal{M}^2(\psi). \quad (2.29)$$

Where,

$$F_{\mu, \theta}(x) = \frac{1}{e^{(x-\mu)/k_B \theta} + 1}. \quad (2.30)$$

Here, θ is the temperature, and μ is the chemical potential. Similarly, electrons moving from all the tip states with energy $\mathcal{E}$ into unoccupied sample state ψ is described by

$$\frac{d}{dt} \sum_k |a_k(t)|^2 = F_{\mu_t, \theta}(\mathcal{E}) \frac{2\pi}{\hbar} \rho_{\text{tip}}(\mathcal{E}) \mathcal{M}^2(\psi). \quad (2.31)$$

Therefore, we have the rate of electron transfer (2.29) from a specific sample state ψ_n with energy $\mathcal{E}_n$ into unoccupied tip states, and the rate of electron transfer (2.31) from all unoccupied tip states into the sample state ψ_n .

Since the system is in chemical equilibrium and the occupation probabilities of the tip and sample are assumed to be independent of each other, at temperature θ and chemical potential μ_s , the probability of an electron existing in the sample state ψ_n with energy $\mathcal{E}_n$ is $F_{\mu_s, \theta}(\mathcal{E}_n)$. Now, summing over all sample states weighted by their occupation probabilities we get the total rate of electron transfer from the tip to the sample and vice versa.

Therefore, the tunnelling current I can be calculated by taking the difference of the two rates of electron transfer and multiplying the result by the charge of an electron e .

$$I = \frac{2\pi e}{\hbar} \sum_n \{F_{\mu_i, \theta}(\mathcal{E}_n)(1 - F_{\mu_s, \theta}(\mathcal{E}_n)) - (1 - F_{\mu_i, \theta}(\mathcal{E}_n))F_{\mu_s, \theta}(\mathcal{E}_n)\} \rho_{\text{tip}}(\mathcal{E}_n) \mathcal{M}^2(\psi_n) \quad (2.32)$$

At low temperatures as ($\theta \sim 0$), equation 2.30 becomes a Heaviside step function. Therefore, the tunnelling current formula simplifies to

$$I = \pm \frac{2\pi e}{\hbar} \sum_{n: \mu_a < \mathcal{E}_n < \mu_b} \rho_{\text{tip}}(\mathcal{E}_n) \mathcal{M}^2(\psi_n). \quad (2.33)$$

Where $\mu_a = \min\{\mu_s, \mu_t\}$, $\mu_b = \max\{\mu_s, \mu_t\}$ and $\pm$ depends on if $\mu_t > \mu_s$ or $\mu_t < \mu_s$. The sum in the tunnelling current equation can also be approximated by an integral, giving us

$$I = \pm \frac{2\pi e}{\hbar} \int_{\mu_a}^{\mu_b} \rho_{\text{tip}}(\varepsilon) T(\varepsilon) \rho_{\text{sam}}(\varepsilon) d\varepsilon. \quad (2.34)$$

Where $T(\varepsilon)$ is the average of $\mathcal{M}^2(\psi_n)$ over all states with energy $\mathcal{E}_n$. However, at chemical equilibrium $\mu_t = \mu_s$.

In 1983, Tersoff and Hamann [31] applied Bardeen's theory to the STM. Chen [4] improved on this, and the currently used tunnelling current equation for STMs is

$$I = \frac{2\pi e^2}{\hbar} |M_{\mu\nu}|^2 \rho_B(E_F) \rho_A(E_F) V. \quad (2.35)$$

Where A and B are the two electrodes, V is the applied voltage, and $|M_{\mu\nu}|$ is the tunnelling matrix element. Here, V raises the electron levels on one side of the tunnelling junction, leading to a net current in one direction, and

$$\rho(E_F) \sim \text{constant} \quad (2.36)$$

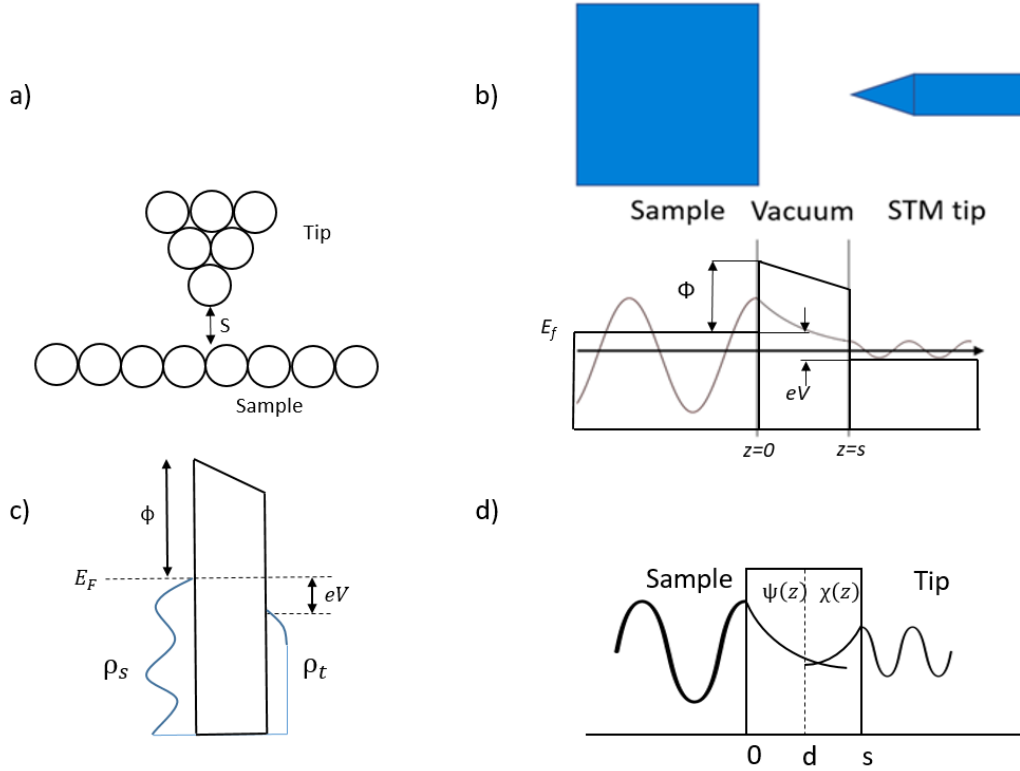


Figure 2.1: The diagram in (a) represents a probe tip and the sample with “ s ” representing the gap between them. Diagram (b) shows the tunnelling effect exploited by the STM and diagrams (c) and (d) show Bardeen’s approach to quantum tunnelling. The integral over the overlap of $\psi(z)$ and $\chi(z)$ in the diagram (d) is used to calculate the tunnelling matrix element M . [4]

Tunnelling Spectroscopy

According to Chen [4] equation 2.35 can be rewritten with the tunnelling matrix element M , bias voltage V and as

$$I = \frac{4\pi e}{\hbar} \int_{-\infty}^{+\infty} [f(E_F - eV + \epsilon) - f(E_F + \epsilon)] [\rho_s(E_F - eV + \epsilon) \rho_t(E_F + \epsilon)] |M|^2 d\epsilon. \quad (2.37)$$

Where $|M|$ is the tunnelling matrix element that describes the spatially integrated overlap of the tip and sample electronic wavefunctions. This is done by summing over all relevant states at a finite temperature.

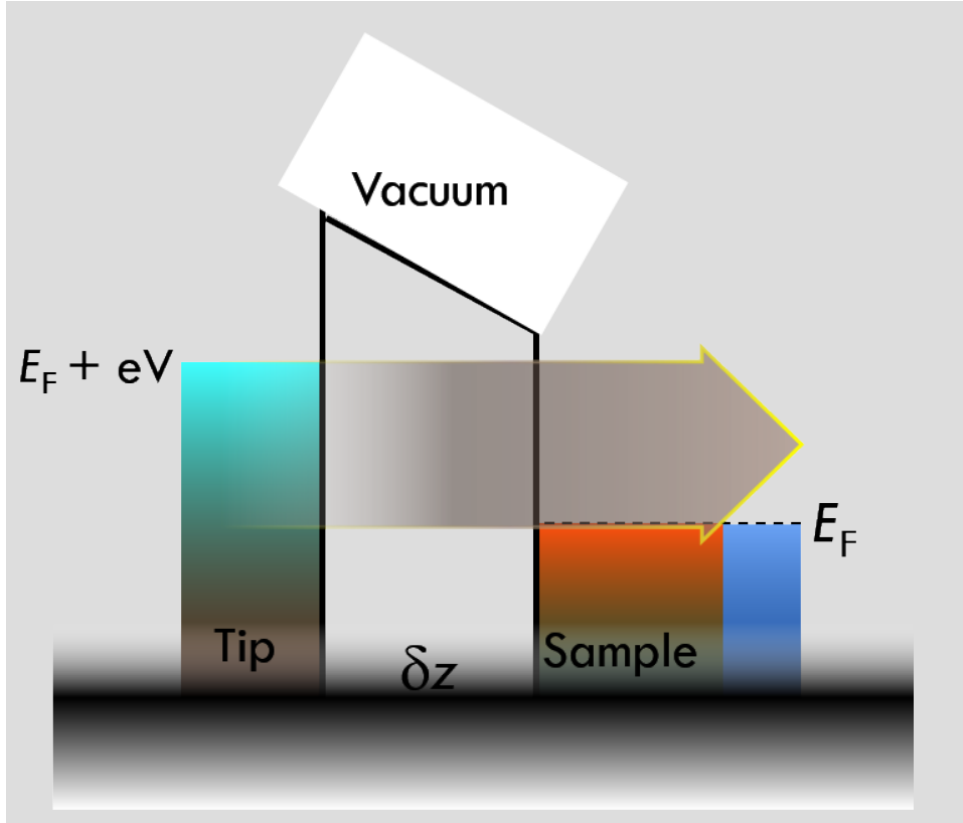


Figure 2.2: The Fermi level of the tip is increased here by the bias voltage (V) providing empty states for the electrons in the sample.

$f(E) = \left(1 + \exp\left[\frac{E - E_F}{k_B T}\right]\right)^{-1}$ is the Fermi distribution function. This allows the calculation of the occupancy of electronic states at temperature T . As T approaches 0 or $k_B T$ is smaller than the energy resolution required in the measurement, the Fermi

function can be treated as a step function, and the current equation can be simplified to,

$$I = \frac{4\pi e}{\hbar} \int_0^{eV} [\rho_s(E_F - eV + \epsilon) \rho_t(E_F + \epsilon)] |M|^2 d\epsilon. \quad (2.38)$$

Bardeen further assumed that the magnitude of the tunnelling matrix is constant in the interpretation of the experiment of Giaever [36] [37]. The details of it for an STM tip were considered by Tersoff and Haman [31] but go beyond the scope of the theory necessary to understand the functional capabilities of an STM or the theory needed to understand most experiments. Therefore, the tunnelling current is just proportional to the density of states of the two electrodes, as shown in 2.39.

$$I \propto \int_0^{eV} \rho_s(E_F - eV + \epsilon) \rho_t(E_F + \epsilon) d\epsilon \quad (2.39)$$

If the tip is approximated as a free-electron metal, the density of states can be treated as a constant. Therefore, from the fundamental theorem of calculus, the rate of change of tunnelling current with respect to bias voltage (dI/dV), the differential conductivity of the junction, is directly proportional to the density of states, as well.

The integral above is integrating from the Fermi level (the highest occupied state) to the bias voltage energy shift. The equation computing the density of states in the corresponding unit energy levels of both the tip and the sample directly ties into Fermi's golden rule for transitions from occupied to unoccupied states in Fermions. Integrating this product from the Fermi Level up to the bias voltage energy shift gives a count of how many states can tunnel, which is proportional to the conductance of the junction.

The primary difference between the one-dimensional case and the three-dimensional case for the Bardeen theory of tunnelling is in the derivation of the tunnelling matrix element $|M|$. Since the details of $|M|$ are beyond the scope of the theory needed for this project, as mentioned before, the three-dimensional case is not discussed here.

2.1.3 Spin-polarized Scanning Tunnelling Microscopy

Spin-polarized tunnelling occurs in a tunnelling junction where the two electrodes are made of magnetic materials (typically ferromagnets). In this case, the tunnelling current's strength depends on the electron spin's relative orientation in both electrodes. The spin angular momentum is an intrinsic property of electrons and has two eigenstates: spin-up and spin-down.

In an STM, if the tip is spin polarised (has the spins of electrons aligned in a specific direction in space), the strength of the tunnelling current will depend on the relative orientation of electron spin in the sample. Figure 2.3 shows a schematically simplified version of a spin-polarized tunnelling junction [38], and according to this representation, the spin-up state is energetically shifted from the spin-down state. This shift leads to spin polarization at the Fermi level.

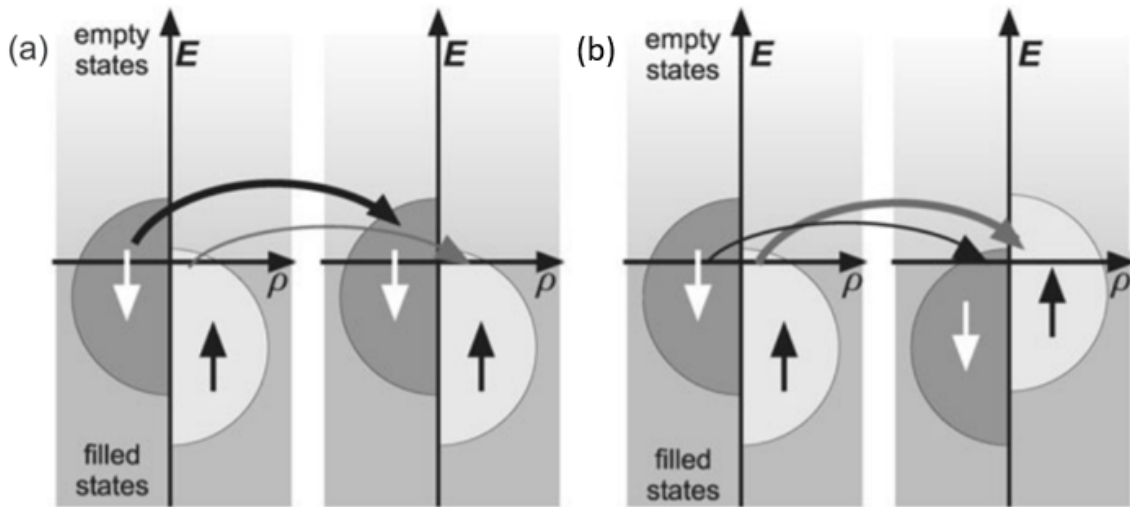


Figure 2.3: Principle of spin-polarized tunnelling between magnetic electrodes that exhibit (a) a parallel and (b) an anti-parallel magnetization. The spin is conserved in the case of elastic electron tunnelling. Therefore, spin-up electrons that tunnel out of the occupied states of electrode A can only enter empty spin-up states of electrode B [39].

A few modifications to Bardeen's theory must be made to understand the theory behind spin-polarized tunnelling. First, the density of states will now have to be split into two components that describe the two eigenstates. The derivations of the matrix elements with spin incorporated can be found in Chen [4]. Finally, we get the equation

for the conductivity with zero bias current as [39]

$$\frac{dI}{dU} \propto \rho_T^\uparrow(E_F)\rho_S^\uparrow(E_F) + \rho_T^\downarrow(E_F)\rho_S^\downarrow(E_F). \quad (2.40)$$

From this “two current model,” initially introduced by Julliere [40], the dependence of conductivity to spin orientation can be described.

2.2 Piezoelectricity

Piezoelectric ceramics are one of the most important technological advancements that enabled the invention of the STM. They help provide all coarse and fine motion in the STM head. The tip and the sample need to be less than a nanometer away from each other for the STM to be able to scan, and this can only be done using piezoelectric crystals. This section will cover the fundamental physics behind piezoelectricity.

2.2.1 Piezoelectric effect and Inverse Piezoelectric Effect

The piezoelectric effect was discovered by Pierre and Jacques Curie more than a hundred years before the invention of the STM [31]. The Curie brothers showed that when mechanical stress is applied to certain crystals, they produce an electric potential. This was called the piezoelectric effect.

A few months later, Lippmann [41] predicted that the piezoelectric effect could be reversed to achieve deformation in a crystal by applying a voltage to it. This was called the inverse piezoelectric effect. The Curie brothers designed an experiment and proved this effect in 1882 [41]. There are many naturally occurring materials that exhibit the piezoelectric effect, such as quartz, topaz, Rochelle salt, etc. Several artificially made materials can exhibit the piezoelectric effect. Lead zirconate titanate (PZT) is one of the most commonly used artificial materials with the piezoelectric effect and is used in nano-positioning systems.

STMs primarily use various kinds of PZT ceramics to achieve precise motion.

PZTs have an enhanced piezoelectric effect due to their permanent electric polarization. They are also only useful in ceramic form for STM functionality, and when they are made, they have a random arrangement of electric dipoles. The as-made PZT ceramics have to go through a poling process to achieve permanent electric polarization, similar to the process of making a permanent magnet. However, this polarized state can be easily reversed by exposing the material to an environment above a specific temperature, and this limit is called the Curie temperature. One of the significant disadvantages of PZTs is that their Curie temperature is very low (200°-400°C).

After the poling process, the PZT ceramics can be a very reliable material for STMs due to their extremely small deformations. These deformations are not continuous, but the step size is small enough to be used in the STM. The tube geometry helps mitigate the effects of the non-continuous deformations and allows the PZT ceramics to be used as scanning probes as well. The only major limitation to the precision of the motion created by these piezoelectric ceramics is the precision of the applied voltage. Another main advantage of piezoelectric crystals is the absence of (translationally) moving parts within them. They could also be made into any basic shape, fitting into the design parameters of the STM flawlessly. They are also ultra-high vacuum (UHV) compatible and work well at cryogenic temperatures. For this project, a tube scanner and shear plate piezoelectric ceramics will be used to produce the required fine and coarse motions, respectively.

The deformation of the piezoelectric materials depends on the electric polarization (P), piezoelectric coefficients (d_{ijk}) and mechanical stress (σ). Similarly, the inverse piezoelectric effect depends on the mechanical strain (ε), piezoelectric coefficients (d_{ijk}) and the electric field applied (E). The following equations can explain the electric polarization and the mechanical strain:

$$\begin{aligned} P &= d_{ijk}\sigma \\ \varepsilon &= d_{ijk}E \end{aligned} \tag{2.41}$$

From these equations, the required piezoelectric constants can be derived as a tensor component d_{ijk} and has a unit of $\frac{m}{V}$.

2.2.2 Tube Scanner

The tube scanner was invented in 1986 by Binnig and Smith [42], immediately becoming the dominant scanner used in STMs. The design of the tube scanner is much simpler than the previous scanners, and it also has high piezo coefficients and resonant frequencies ($\sim 8kHz$). The tube scanner (shown in Figure 2.4) is made of PZT with a metal coating on the inner and outer surfaces. The PZT is radially poled and divided into four quadrants to provide the x and y directional motion. This is done by applying a voltage to extend one of the quadrants while contracting the opposite quadrant to make the tube bend in one direction. One of the main disadvantages of the tube scanner is that the x, y and z motions are non-linear and are not precisely orthogonal, but this can be fixed with a suitable controller, programs and hardware. As the x and y directional motion is achieved by the bending of the tube, it can also be approximated as continuous motion.

The deflection in the x and y direction can be calculated geometrically, assuming the stress generated only affects one direction. This deflection is a function of the voltage applied (V) and is derived as:

$$\Delta x = \frac{2\sqrt{2}d_{31}L^2}{\pi Dh}V \quad (2.42)$$

$$\Delta y = \frac{2\sqrt{2}d_{31}L^2}{\pi Dh}V \quad (2.43)$$

And the z -directional motion can be derived to be:

$$\Delta z = V \times \frac{d_{31}L}{h}. \quad (2.44)$$

Where d_{31} is the piezoelectric strain constant, L is the length of the piezoelectric tube, h is the tube thickness, and D is the outside diameter of the tube.

The piezoelectric strain constant can be measured by applying an AC voltage to both the y quadrants of the tube scanner and measuring the voltage and current produced by the x quadrants due to the inverse piezoelectric effect. Then the following equation

provides the piezoelectric strain constant.

$$d_{31} = 45.0 \sqrt{\frac{\bar{I}h}{f\bar{V}DLY}} \quad (2.45)$$

Where $\bar{I}$ is the measured current, $\bar{V}$ is the measured voltage in the x quadrants, Y is Young's modulus of the piezoelectric ceramic and f is the frequency of the applied AC voltage.

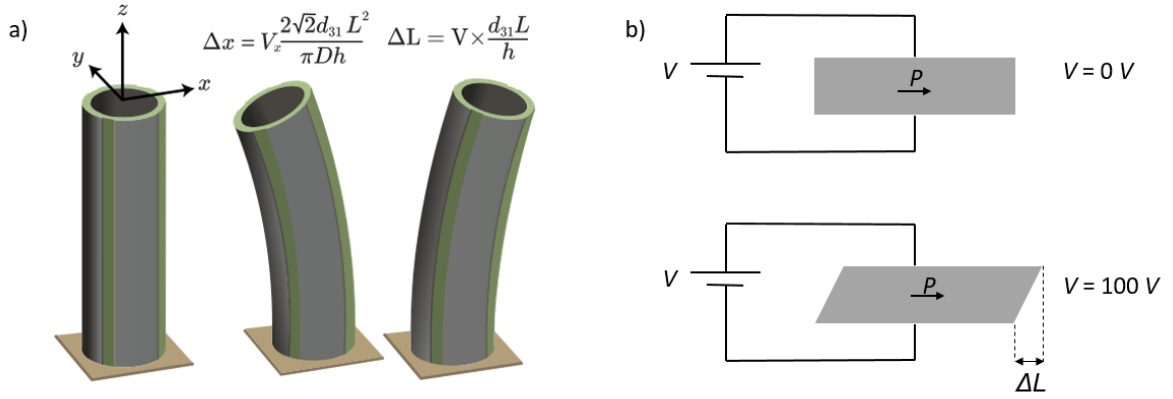


Figure 2.4: A tube scanner with how the x and y motions are obtained is shown in (a) [43], with the equations used to calculate the displacements. Shear piezo with its lateral deformation and the polarization direction is shown in (b).

2.2.3 Shear Plate Piezoelectric Ceramic

Shear plate piezoelectric ceramic or, in short, shear plate piezos are used for all coarse motion in the STM head. These piezos allow us to bring the STM into the scanning position so that the tube scanner can take over for the scanning process.

The deformation ΔL is caused in a shear plate piezo is shown in Figure 2.4 when a voltage difference is applied across it. This deformation can be calculated using the equation:

$$\Delta L = d_{15}\Delta V \quad (2.46)$$

Where d_{15} is the piezoelectric constant and ΔV is the voltage applied. The piezoelectric constant is the ratio of the deformation length (ΔL shown in Figure 2.4) over the change in the thickness of the shear plate piezo when an electric field is applied across it. Here the applied mechanical stress is shear and is at right angles to the original poling electrodes.

These shear plate piezos are made by applying very high voltages across them ($\sim 40kV$) and then cut into plates [4]. Therefore, the voltage applied to these piezos must be kept below the depolarizing limit to maintain their stability and life.

In both the Shear plate piezo and the tube scanner, the piezoelectric constants are the ratio of the component of the strain tensor over the applied electric field intensity in the respective direction. The discovery and improvements of the piezoelectric crystals is what made the invention of the STM possible.

Chapter 3

Design and Analysis

The STM is an instrument that was born when various branches of science and technology that communicated little with each other were brought together [44]. Major design challenges had to be dealt with to produce a stable tunnelling junction that could scan with atomic resolution for the invention of the STM.

One of the fundamental challenges with the STM design is the movement and positioning of the scanning tip. This is primarily done using piezoelectric materials that can deform when a voltage is applied. Due to the scale of these deformations being in the nanometer scales, they become the ideal material for making STM head motors. Most of the major design breakthroughs and improvements for the last four decades since the invention of the STM come from the improvement of the piezoelectric motor designs. However, the fine motion motor of the STM head has been mostly standardized to use the tube scanner introduced in Chapter 2. Therefore, all the design focus has shifted to the coarse motors in the STM head.

The original STM invented by Binnig and Rohrer followed a tripod design, as shown in Figure 3.1. In this case, there is a primary piezoelectric slab that can expand and contract when a voltage is applied. It rests on three metal feet separated by insulators from the ground plates. The piezoelectric slab can be clamped to the metal feet by applying a voltage between them.

This mechanism, nicknamed the louse, works by clamping two of the three metal

legs and applying a voltage to the piezoelectric slab to make it expand or contract. This moves the piezoelectric slab on the third unclamped leg. Then, the third leg is clamped, the original two clamped legs are unclamped, and the voltage applied to the piezoelectric slab to move in the two original legs is removed. This process allows the mechanism to take one step, and the step is between 10 and 100 nm [45]. As the piezoelectric slab can be clamped to one leg and rotated around it, the slab can move in any given direction.

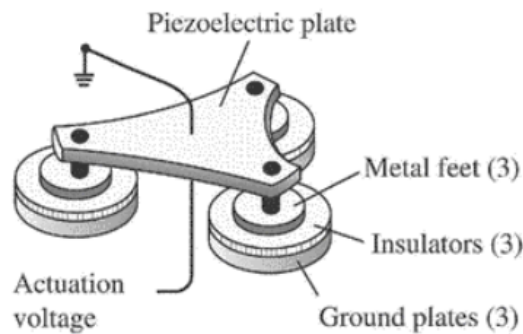


Figure 3.1: Diagram of the original STM head design created by Binnig and Rohrer. This design features a piezoelectric plate that can expand when a voltage is applied to provide all the required motion. This diagram is taken from C. Julian Chen, Introduction to Scanning Tunneling Microscopy 3E © 2021 Oxford University Press Canada. Reprinted by permission of the publisher [4].

This was the primary design philosophy that was followed by STM heads until the invention of the single-tube three-dimensional scanner [46]. Using a tube scanner allows the STM head to have a much smaller footprint and also allows the resonant modes of the head to be much higher since the lowest mode of the tube is around 8 kHz. The tube scanner also allows for faster scans and provides more reliable, smaller and simpler STM heads [46]. Since its invention, the tube scanner has become the standard fine-motion motor in STM heads. The anatomy and theory behind the tube scanner are explained in Chapter 02.

3.1 Types of STM heads

As the fine-motion motor has been standardized for STM heads, major changes and improvements have been coming from the coarse motor designs. Some of the historically significant designs are the single-tube STM, the Besocke-type STM, the Pan design and the inchworm. The louse design was the first successful STM to be used in Ultra-high Vacuum (UHV). Most modern commercial and homemade STMs are designed around the tube scanner.

3.1.1 The Besocke-type: the beetle

Invented in 1987 by Besocke [47], this design has been used by various laboratories around the world as the basis for their STM and AFM designs. This design consists of four tube scanners, as shown in figure 3.2. The three outer tubes are responsible for the coarse x, y and z directional motion, and the centre tube controls the fine motions in the three dimensions. Since the tube scanners are made of identical materials and due to the nature of the design, this type of STM has low thermal drift and minimum vibrations.

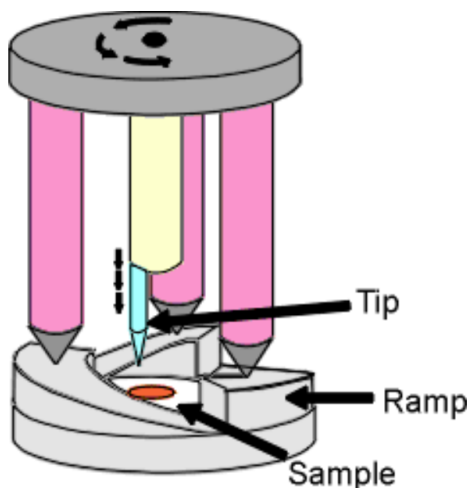


Figure 3.2: Diagram of a typical Besocke-type STM scan head. The three pink scanning piezoelectric tubes are used for coarse motion, while the central yellow piezoelectric tube is used for fine motions [48].

The tube scanners provide the required xy motion for the STM using the stick-

slip procedure discussed in Chapter 2. The z -directional motion is achieved using the ramp in the base as the tube scanners walk up on them. The identical coarse and fine motion tube scanners expand and contract the same amount with the temperature changes, cancelling any thermal drift. Having identical tubes with the same speed of sound makes them less susceptible to external vibrations [44].

Since there are no spring forces helping the stick-slip motion in this design, the head has to be heavy to provide the required normal force for this motion and reduce the rocking vibrations of the STM head. The high mass of the head introduces some significant disadvantages to this design, including the reduction in the frequency of spring pendulum modes and internal modes of the head, causing low-frequency vibrations. This also interferes with data collection as data acquisition is done at low frequencies in the STM head. To compensate for this, we would need to increase scan times, which goes against one of the primary goals of this project. Another major drawback of this design is that the motion produced by the coarse tube scanners is non-linear, and the x and y motion is not precisely orthogonal. Therefore, this project did not choose the Besocke type as the basis for STM head design.

One important STM head design that came from the Besocke type is the variable temperature STM developed by Wilson Ho's group [49], shown in Figure 3.3. In this design, the STM assembly is mounted on an optics table with pneumatic legs to filter out any high-frequency vibrations, and the STM head is suspended with three springs with eddy-current damping to filter out the low-frequency modes. This design allows atomic resolution even when the temperature is not constant.

The temperature is varied using a continuous-flow cryostat in this STM. The primary difference between this STM and a conventional Besocke-type STM is the way xy scanning is done. Here, the outer tube scanners are used for xy scans instead of the central tube. The central tube scanner is used only for z directional motions.

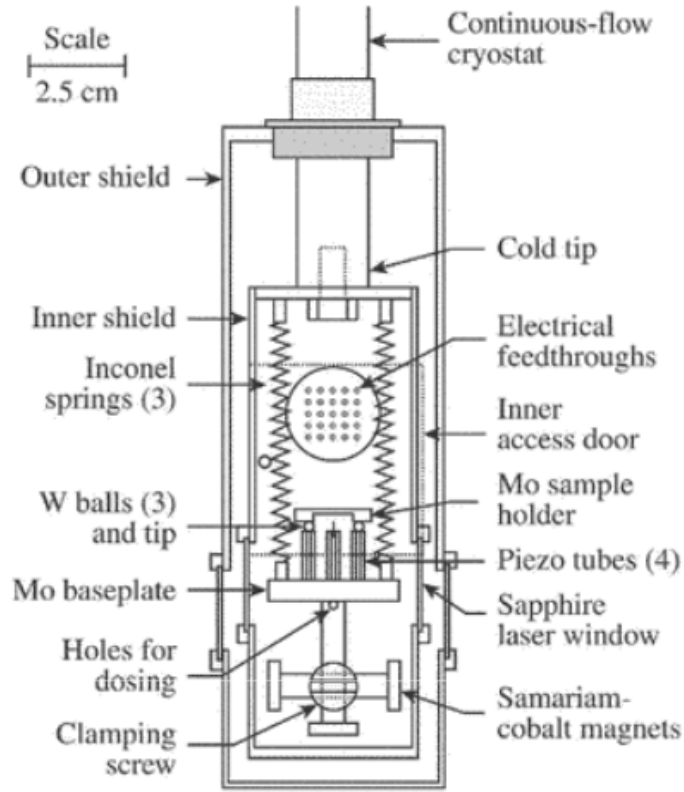


Figure 3.3: In the variable temperature STM head a continuous flow cryostat is used to cool the head. Vibration isolation is done in two stages, first by placing the UHV chambers on an optical table with pneumatic legs and then suspending the STM head on three springs with Eddie current damping for the second stage filter. This diagram is taken from C. Julian Chen, Introduction to Scanning Tunneling Microscopy 3E © 2021 Oxford University Press Canada. Reprinted by permission of the publisher [4].

3.1.2 The Pan Design: Walker

S. H. Pan developed the Pan design [7], which is ideal when high rigidity and stability are crucial. It is also the primary choice for cryogenic temperatures and UHV scans. This design simplifies the scan head by moving the coarse x and y motions to the sample holder, as shown in Figure 3.4. The coarse motion in this design is done using shear plate piezoelectric stacks instead of tube scanners. As shown in Figure 3.4(a), the STM head consists of a prism that holds the tube scanners for the fine motions, and the prism is

held inside a cage by the piezoelectric stacks with a spring plate providing the tension required to hold the prism in place. There are six piezoelectric stacks for the coarse z motion.

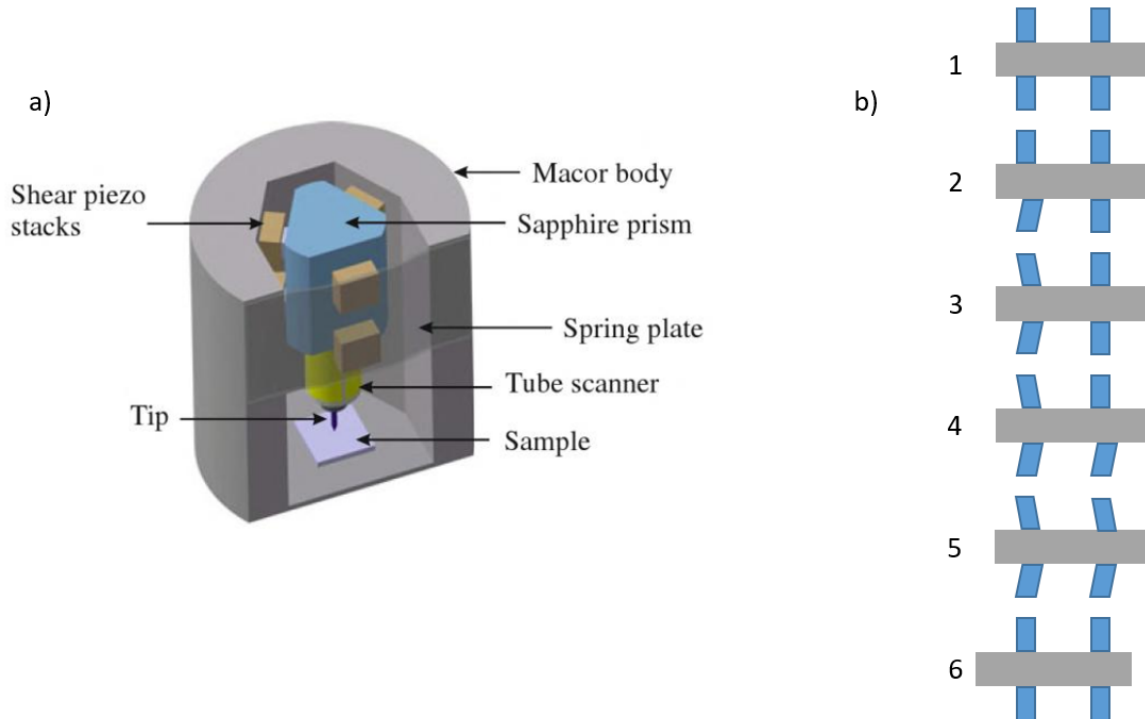


Figure 3.4: a) A typical Pan style STM head [50] with the prism tensioned by a spring plate. Reprinted by permission of the publisher. b) Shows the mechanics of stick-slip motion with the piezos (blue) deforming and moving a plate (grey). The six steps shown here take place in sequence and make one step of the stick-slip motion.

The coarse z motion is achieved using the stick-slip process, as shown in Figure 3.4(b). This is a simplified model showing only four stacks. In this case, the voltage applied to the piezoelectric stacks is initially ramped up slowly to bring them to their deformed position, which is done to one stack at a time. Once all the stacks are in their deformed position, the voltage is cut off so that the piezoelectric stacks move the prism in the corresponding direction. This provides one step of the motion, and the repetition of this procedure provides the coarse z-directional motion. A similar process is used for coarse x and y motion as well.

One significant disadvantage of the stick-slip motion is the friction between the piezoelectric stacks and the sides of the prism. This can wear out the top of the

piezoelectric stacks or the sides of the prism extremely fast. One solution to this problem is to add a layer of very hard material to the tops of the piezoelectric stacks and the sides of the prism. One of the most commonly used materials is Alumina Oxide.

The STM head for this project is based on the Pan design. The Pan design's primary advantages- such as high rigidity, UHV compatibility and the ability to work at cryogenic temperatures- align with the goals of this master's thesis.

3.2 Design tools and programs

Autodesk Inventor was the primary computer-aided design (CAD) program used for all STM designs in this project. CAD software provides 3D mechanical design, documentation, and simulation tools [51]. The inventor's work process starts with 2D sketches that are later extruded to become 3D models. These 3D models can subsequently be put together in the Assembly environment of Inventor to make the final apparatus. This process allows us to visualize and solve design problems in the early prototyping stages. Autodesk Inventor also allows the designs to be exported in various formats for the production process, further analysis or collaboration with other projects.

One of the primary goals for the STM head is to have high resonant modes, and this was done by exporting the models to the NASTRAN environment of Autodesk Inventor and running simulations in it. NASTRAN is a finite element analysis program developed by NASA in the '60s for their aerospace program [52]. It is now integrated into various software packages in a wide variety of fields. NASTRAN is considered the industry standard for computer-aided engineering for all types of structures [53].

3.3 The Design

The primary design goals of this project are to build a functioning STM head, minimize its $z(t)$ vibrations, and maximize the resonant frequencies, UHV compatibility and non-magnetic components. In this case, $z(t)$ is the distance between the sample and the

end of the STM tip as a function of time. High resonant frequencies will minimize the effect of normal modes on long scans. UHV compatibility is necessary as the head will be placed in a UHV chamber for scans. UHV environment improves the performance of STMs. Non-magnetic components will help study magnetic samples without applying stray magnetic fields to the samples.

The reason for the requirement of high resonant frequencies is that most of the high-frequency vibrations are filtered out of the STM. This is done by suspending the STM head using beryllium copper extension springs with low coupled spring pendulum modes (8-10 Hz), preventing higher frequency vibrations. Therefore, designing the STM head to have high-frequency vibrational modes will mismatch with the low-frequency modes passed through the springs and make the design very rigid and vibrations resistant.

Aluminum was chosen as the primary material for the components as some of the design requirements for the parts were that they be as light as possible, have high vibrational modes and be non-magnetic to study magnetic samples. The machinability of aluminum is also a great advantage. The design should also be UHV compatible. Thus, all the holes in the parts must be through holes so that no air pockets are trapped as the STM is placed in the UHV chamber. This also helps dampen any eddy currents in the components.

Appendix A contains detailed drawings of all the components in the STM head. The drawings include all the required dimensions for recreating the parts.

3.3.1 Z Motor Assembly

The Z Motor Assembly is the part of the STM head where coarse z motion and all fine motion are performed. It consists of the prism, prism cage, cage inserts, prims hat, piezoelectric tube scanner, tip holder, tube insulator, and the STM tip, as shown in figure 3.5.

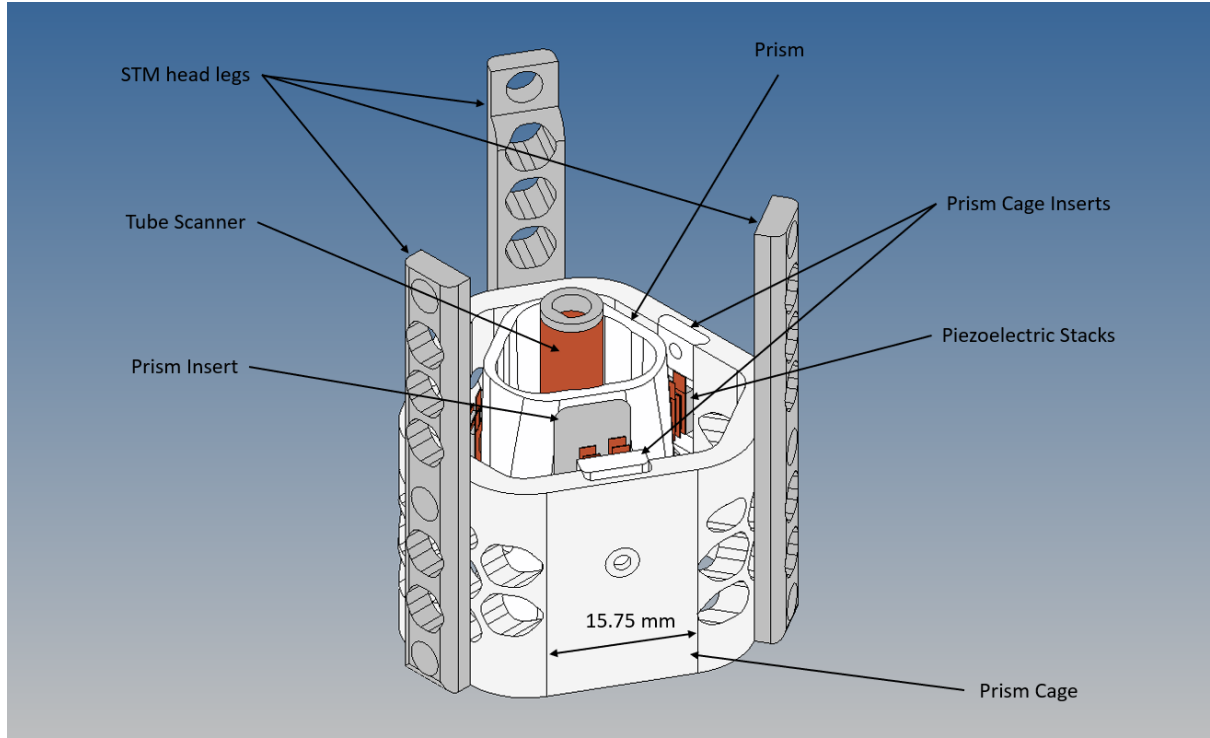


Figure 3.5: Z Motor Assembly of the STM head with its components and the STM legs that connect it to the sample stage.

Prism

The prism is the only component in the Z Motor Assembly design with translational motion. The design is similar to the Pan design, where shear plate piezoelectric stacks hold the prism on all three sides. However, one of the sides has beryllium copper springs behind the piezo stacks to provide the frictional force required for the prism to be held while not moving, as shown in Figure 3.8. As the prism is not directly attached to the rest of the STM head and is held by friction from the piezoelectric stacks alone, it can be moved using the stick-slip motion discussed in section 3.1.2.

In most Pan designs, the prism is made of very hard materials like sapphire [1], [54] or specially coated steel [55] to avoid wear and tear from the constant scratching from the stick-slip motion. However, the weight of these materials and the magnetic properties of steel make it unsuitable for this project. In this design, the prism is machined out of aluminum, and the issue of wear and tear is dealt with by adding alumina slabs to the sides of the prism to provide a hard surface. The piezoelectric stacks are capped

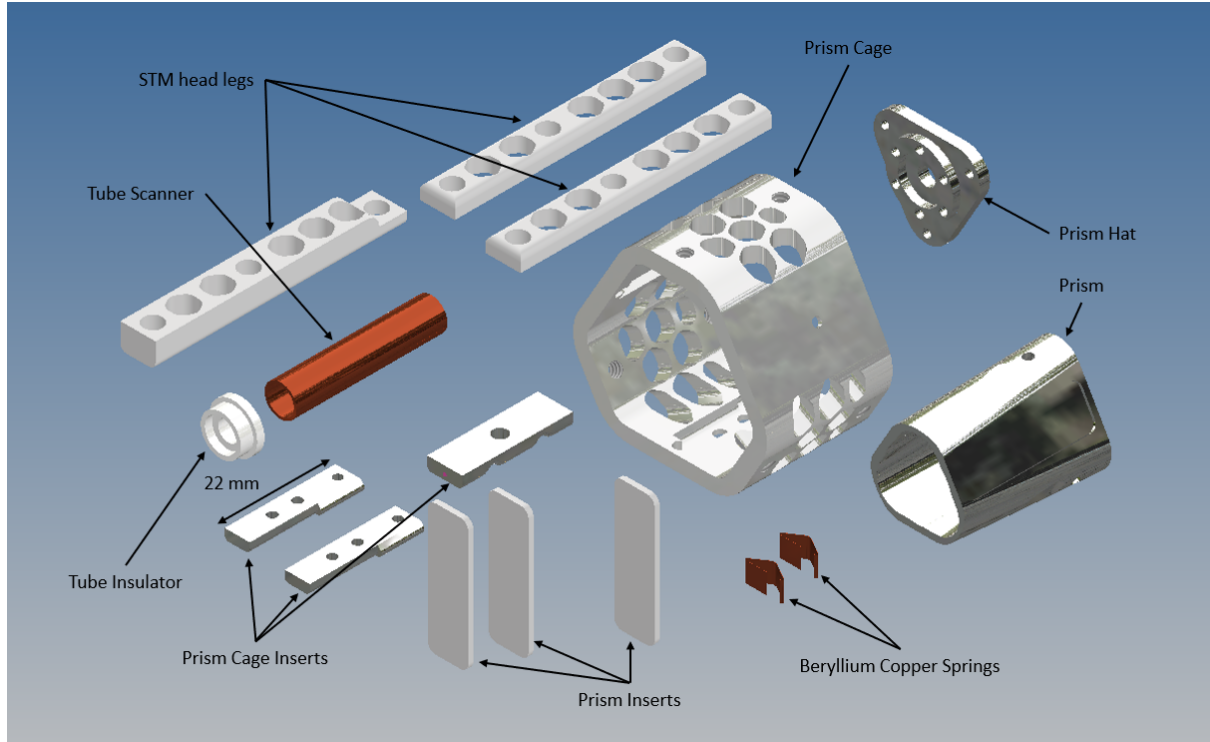


Figure 3.6: Z Motor Assembly of the STM head with its components in an exploded view.

with a sapphire crystal to prevent wear on its side. The low cost of aluminum stock and the machinability of aluminum allowed us to test much more complex designs for the prism. Aluminum is also lightweight and has excellent thermal properties. Finally, the non-magnetic nature of aluminum made it the ideal source for this version of the STM head.

The prism is designed with an open top so the tube scanner can be wired outside the STM head and inserted later into the prism. This design also allows for easy switching of the tube scanner. The prism hat is attached to the prism using 2-56 sized Ti screws. All the screw holes in the prism are vented for UHV compatibility. The range of the coarse z motion depends on the length of the alumina insert in the prism. This version of the STM head allows for about 1 cm of coarse motion.

One of the previous versions of the prism had honeycomb pattern holes to reduce mass while preserving rigidity and increasing the resonant modes. However, after fabrication, it was noted that this design made the prism much weaker to handle, and any excess force applied to it while assembling could deform the prism. Therefore, the

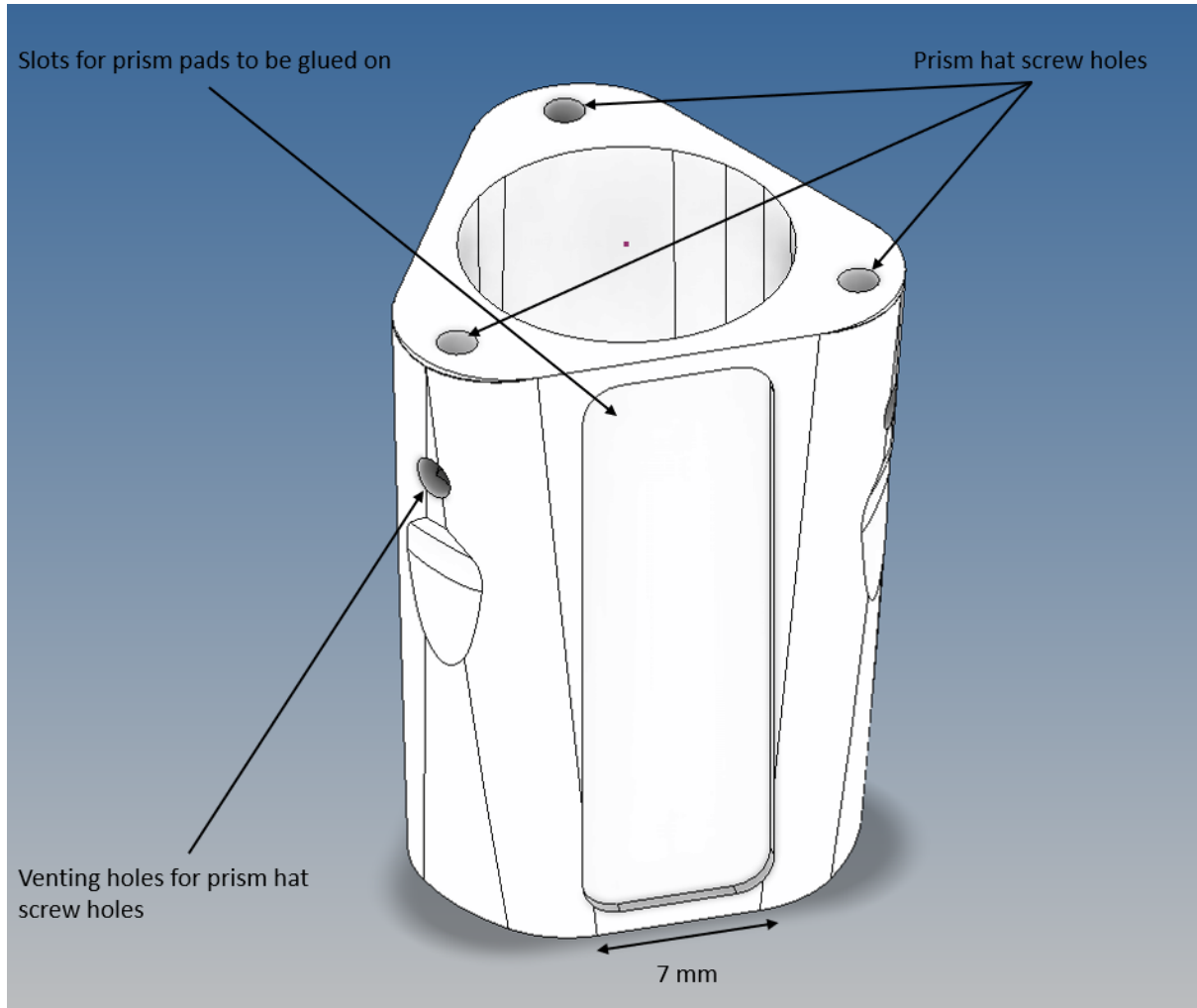


Figure 3.7: Design of the prism with slots for the prism pads to be glued on and the screw holes for the prism hat to be attached shown.

honeycomb pattern was dropped from the prism.

Prism Inserts

Prism inserts are 0.04 in slabs of alumina oxide that were cut into the shape of the slots in the prism to be inserted to avoid wear from the stick-slip motion of the piezoelectric motors. These inserts are glued onto the prism using EPO-TEK H74 UHV-compatible epoxy, and the hardness of alumina will reduce wear and tear.

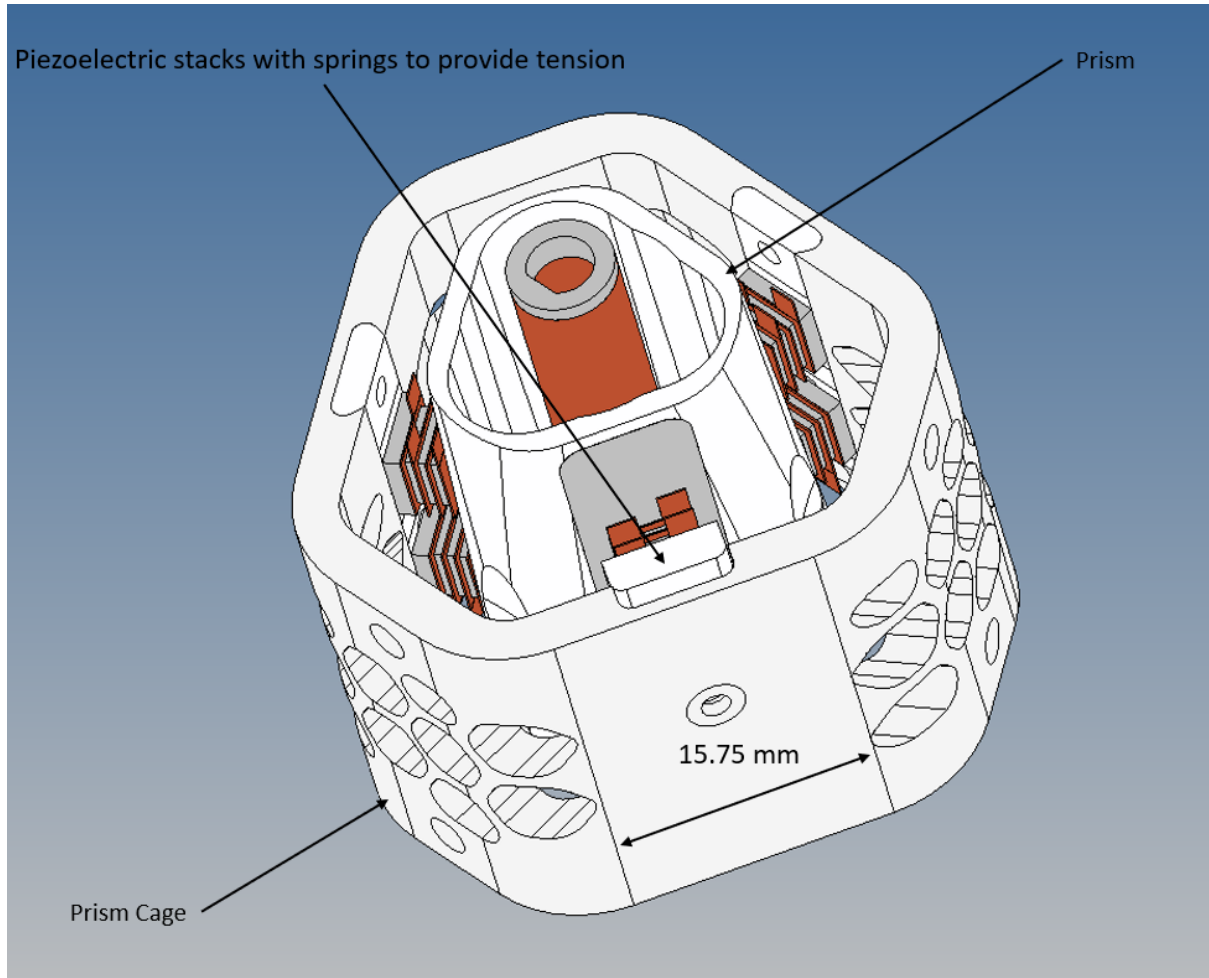


Figure 3.8: Prism being held by piezoelectric stacks with tensioning force applied by beryllium copper springs placed behind the cage inserts.

Prism Cage

The prism cage is the most substantial part of the Z Motor Assembly assembly; it holds all the other parts together. The primary design objectives of this part are to minimize size and mass while maximizing rigidity.

The design is influenced by the Pan-style STM built by B. Drevniok [56]. However, the design was changed into a unibody design, machined out of a single block of aluminum 6061 for better rigidity and reduced mass. The prism cage follows the shape of an equilateral triangle; therefore, the three walls are sixty degrees with respect to each other, as shown in figure 3.9. Dovetail inserts are machined into two of the three walls for inserts with the piezoelectric stacks to be added, and a slot is machined on the remaining

wall for the third piezoelectric stack insert with beryllium copper springs inserts to be inserted. There are screw holes in the inserts and the sides of the prism cage for the inserts to be locked in place. The holes will use 4-40 Ti screws and help improve rigidity in the design. The honeycomb pattern holes on the prism cage help reduce mass while preserving rigidity.

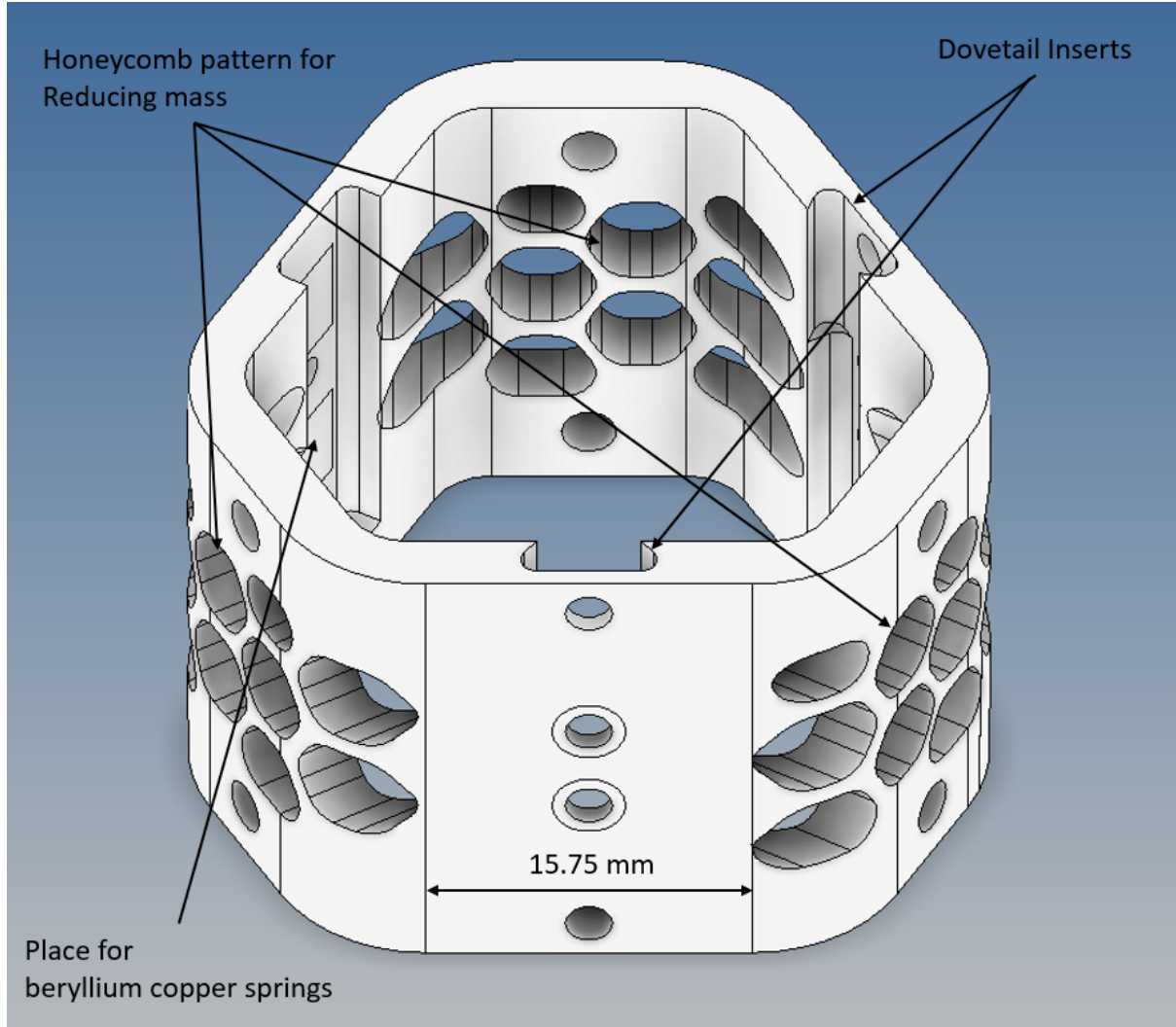


Figure 3.9: Prism cage design with the dovetail slots for cage inserts to be added with piezoelectric stacks and honeycomb pattern cut into the solid walls to reduce mass while preserving rigidity.

The mirror-symmetric design is well-suited for temperature insensitivity. The polished surfaces reflect infrared radiation and help the STM head reach cryogenic temperatures (targeted around 10 K). This prism cage is 38 mm wide, 35 mm long, and 25 mm tall, similar in dimension to other STM heads built before [1], [57], [58].

Prism Cage Inserts

The shear plate piezoelectric stacks are attached to slabs of aluminum that act as a removable component between the prism cage and the stacks, unlike conventional STM head designs [1], [56]. This design allows for the easier wiring of the piezoelectric stacks and the easy replacement of damaged stacks without having to replace the prism cage. The inserts have three holes, two for the screws to fix the inserts in place and the third for any future wire pass-throughs. The insert with the beryllium copper springs has notches for the springs to register against and a screw hole to keep the insert fixed in two dimensions. All the inserts are machined out of Aluminum 6061.

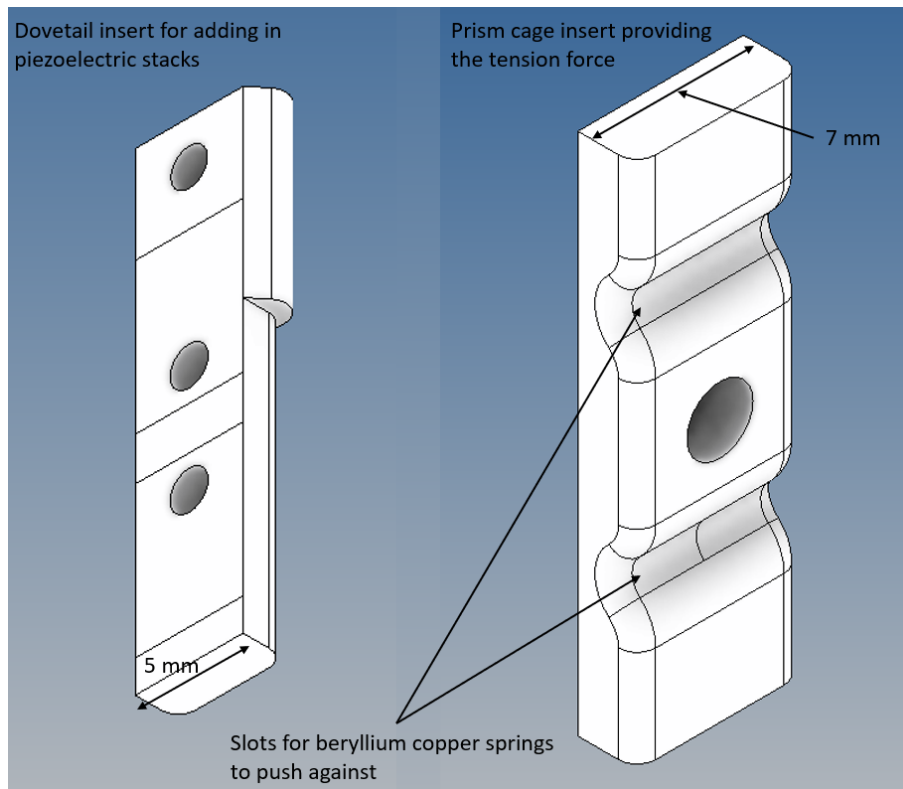


Figure 3.10: Prism cage inserts are used as a platform to add or replace piezoelectric stacks. Cage insert 01 has a dovetail shape and screw holes to be fixed in place. Cage insert 02 has slots for beryllium copper springs to push against and provide the required tension for the prism and a through hole for a screw to help prevent any lateral motion.

Tip Holder, Tube Insulator and Prism Hat

The prism hat is designed to hold the piezoelectric tube scanner outside the prism and improve the accessibility to the tube scanner for wiring purposes. Once all the wiring is completed and the STM tip is added to the prism hat, it can be carefully added to the prism and screwed in place. The prism hat is machined out of aluminum 6061 as well.

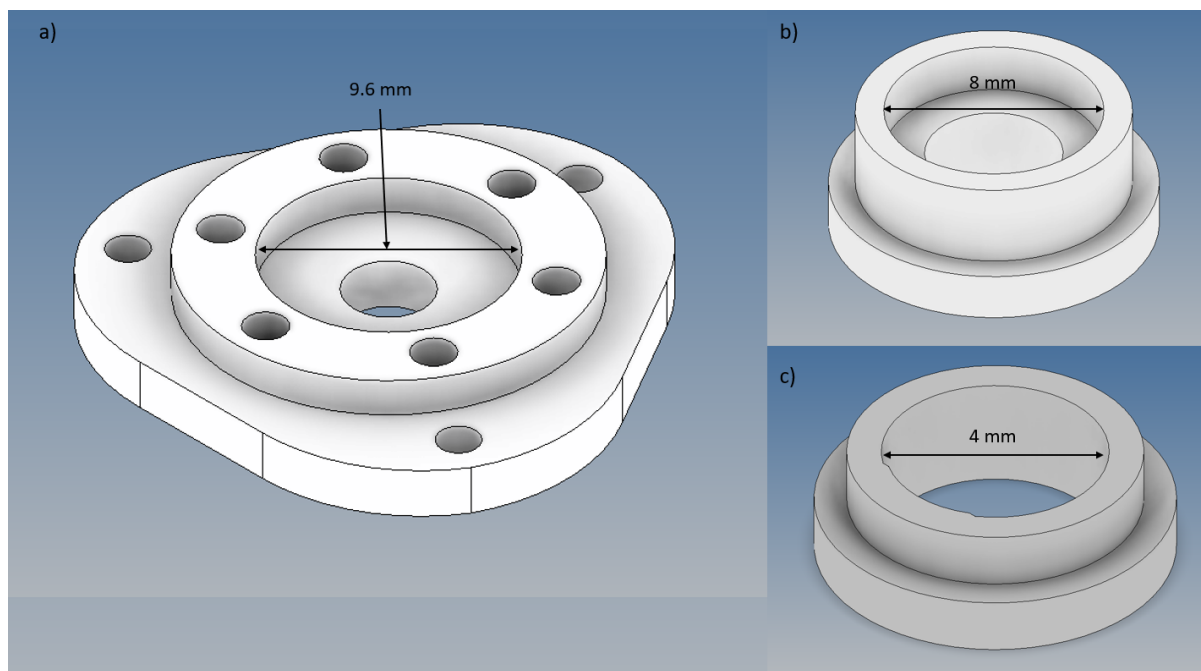


Figure 3.11: a) Prism hat is the platform to which the scan tube is added so it can be wired outside the scan head. This also allows for the easy replacement of the tube scanner. b) The job of the tube insulator is to act as an electrical barrier between the prism hat and the tube scanner and is made of MACOR. c) The tip holder also acts as an insulator between the tube scanner and the STM tip and is responsible for holding the tip in place.

Since the prism hat is conductive, an insulating barrier is needed between the prism cap and the tube scanner. The tube insulator does this. The tube insulator and the tip holder are made out of MACOR. Initial prototypes were machined; however, this was replaced with MACOR washers from McMaster-Carr to reduce mass and machining time. MACOR is a machinable glass ceramic developed by Corning Inc., which is an excellent thermal and electrical insulator (stable up to 1000° C) with very little thermal expansion and UHV compatibility [59].

The tip holder and the tube insulator are designed to be glued into place using EPO-TEK H74 UHV-compatible epoxy.

STM Head Legs

The STM head legs connect the scanning head to the sample stage. This part had a significant amount of mass that could be reduced, and it went through multiple prototypes before the design was finalized. The beryllium copper springs from which the STM head will be suspended attach to these legs at the sample stage. The honeycomb pattern cut into the STM legs helps reduce mass while preserving rigidity.

3.3.2 Sample Stage

The sample stage part of the STM head assembly contains the coarse xy stage. It also contains a sample tray that clips in using beryllium copper leaf springs and is easily replaced with new samples for scanning. Like the Z Motor Assembly parts, most components of the sample stage are machined out of aluminum 6061.

The Sample Cage

The sample cage is the structural frame of the sample stage, containing all the other parts. It is a unibody design, machined from a single block of aluminum for high rigidity and structural stability. The sample cage also contains beryllium copper leaf springs and piezoelectric stacks that provide x-directional coarse motion. Windows are present on the sides of the sample cage to increase the range of y-directional motion. The sample cage will connect to the STM head using 6-32 Ti screws.

Top Plate

The top plate sits inside the sample cage, held by piezoelectric stacks on one side and beryllium copper leaf springs on the other side. This allows the top plate to be moved in

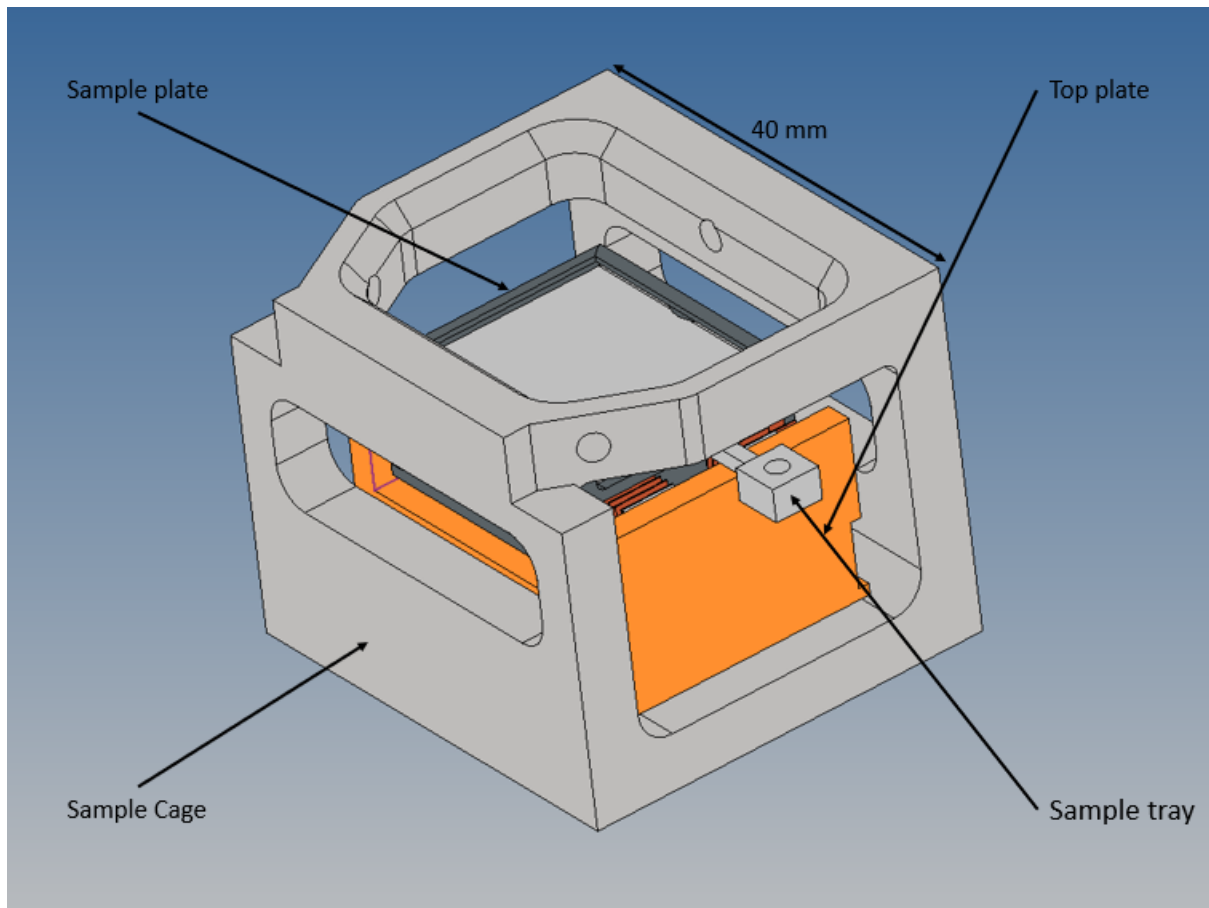


Figure 3.12: The sample stage of the STM head where all the coarse x and y motions will take place. All parts are made of Aluminum 6061 except for the piezoelectric stacks.

the x-direction using the piezoelectric stacks. The size of the piezoelectric stacks determines the thickness of the top plate. Therefore, mass was reduced by having a hexagonal hole in the middle of the plate. The top plate also has its own set of piezoelectric plates and beryllium copper leaf springs to provide y-directional motion.

Sample Plate

The sample plate acts as a connector between the top plate and the sample tray. This design was chosen so that there was a fixed part on top of the top plate for y-directional motion, and the sample could be easily swapped without interfering with the coarse motors. The sample plate has a slot for the sample tray to slide in, and beryllium copper leaf springs clip it in, holding it in place for scans. This was one of the most complex parts of the machine due to its narrow flanges that hold the sample tray.

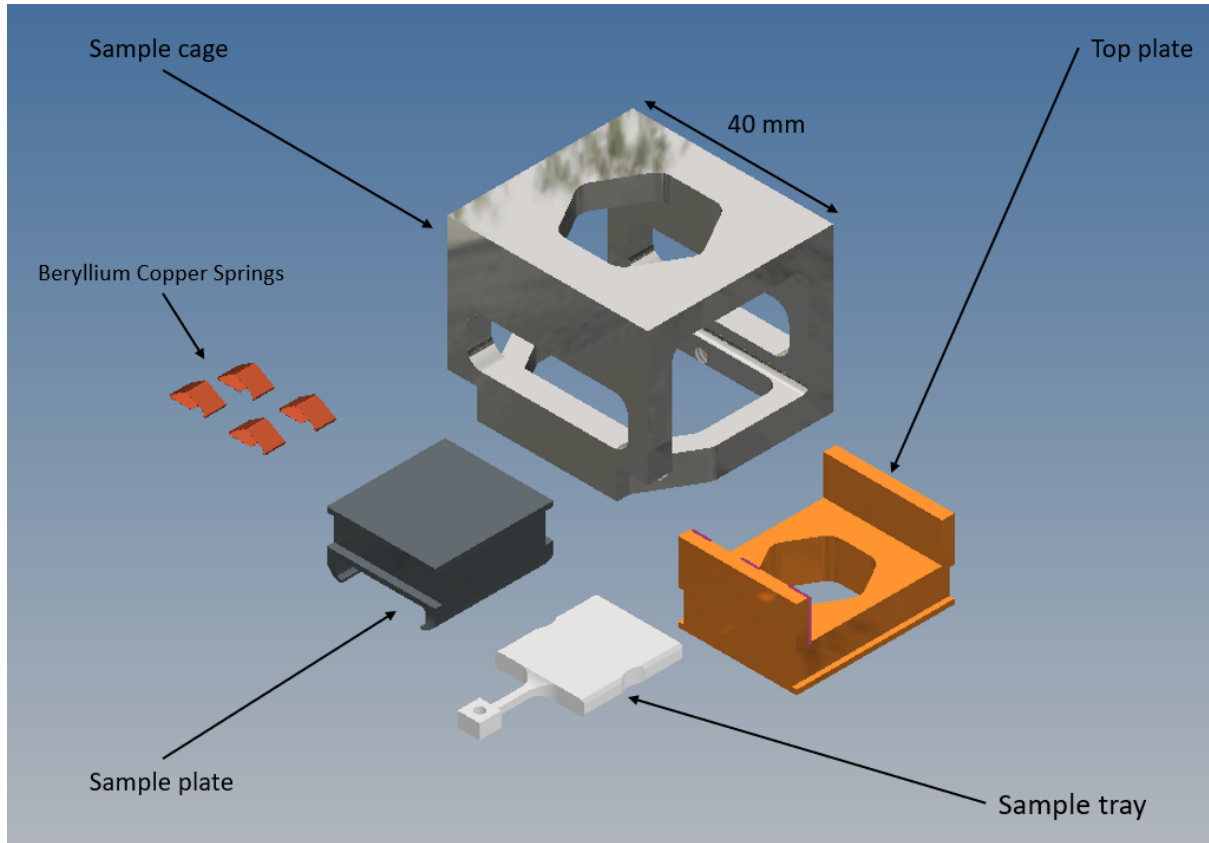


Figure 3.13: The individual components of the sample stage that help provide x and y directional coarse motion.

Sample Tray (Sample Holder)

The sample holder is supposed to hold the samples for scanning with the STM. The current design (sample tray) is generic and has a rectangular space for the samples to be attached to. However, the sample holder will be modified and made custom for each sample depending on the requirements for the sample to be attached. The overall tray design will, however, stay the same so that the sample tray is able to be held by the sample plate using beryllium copper leaf springs. There are notches on the sides of the sample tray for the springs to register.

Another prominent feature of the sample tray is that the handle is designed to be grabbed by the wobble stick in the UHV chambers. This allows samples to be swapped while the STM is under UHV and helps prevent the samples from being exposed to air after being prepped for scanning.

3.4 Finite Element Analysis (FEA)

The finite element method is a numerical way of solving differential equations. This is used by NASTRAN to calculate stress and normal modes on the STM head. FEA was initially developed to study structural mechanics but later expanded to other solid mechanics, heat transfer, fluid dynamics and electromagnetism [60]. One of the main reasons for FEA's popularity among engineers and scientists is the ability to use it in computer programs to solve practical problems.

NASTRAN was used throughout the design process for the normal mode analysis on the STM head, helping to determine various design choices. NASTRAN uses FEA to analyze and calculate the normal modes of parts and assemblies in Autodesk Inventor. Initially, the normal modes of individual parts were calculated and maximized during the design process. Then, all the parts were assembled to make the STM head, and the assembly's normal modes were calculated and maximized. Figure 3.15 shows the first two normal modes of the final prototype and the displacement caused by them.

The fundamental idea behind FEA is to discretize a complex system by dividing it into a mesh of smaller elements called finite elements (FEs) and to identify the degrees of freedom (DOFs) that describe their behaviour. The equations that describe each element's behaviour and interactions with neighbouring elements are assembled into a system of differential equations, which can be combined to obtain the solution for the entire system. The size of the individual element determines the accuracy of the results.

Resonant mode calculations using FEA start with the equation of motion. However, a reduced form of the equation is needed to calculate the natural frequencies. When there is no damping or applied load, the equation of motion is simplified to

$$[M]|\ddot{u}| + [K]|u| = 0 \quad (3.1)$$

where

M = mass matrix

K = stiffness matrix

This equation is for undamped free vibration. It can be solved by assuming the harmonic solution form

$$u(t) = u' e^{i\omega t} \quad (3.2)$$

where

u' = the natural modes independent of time

ω = is the circular natural frequency

This equation is the key to the numerical solution of calculating the natural frequency. Differentiating it with respect to time gives us

$$\ddot{u}(t) = u'(-\omega^2) e^{i\omega t} \quad (3.3)$$

Substituting 3.3 into 3.1 gives

$$-[M](\omega^2)u' e^{i\omega t} + [K]u' e^{i\omega t} = 0 \quad (3.4)$$

$$\therefore e^{i\omega t}([K] - \omega^2[M])u' = 0 \quad (3.5)$$

Since $e^{i\omega t} \neq 0$,

$$([K] - \omega^2[M])u' = 0 \quad (3.6)$$

Since this is a set of linear homogeneous equations, there is a solution only if

$$|[K] - \omega^2[M]| = 0 \quad (3.7)$$

In general, 3.7 is a set of n algebraic equations, where n is the number of degrees of freedom.

The vibrations from the normal modes can cause elastic waves to propagate through the solids, causing elastic deformations [61]. The Navier-Cauchy equation describes the propagation of elastic waves.

$$\rho \ddot{\mathbf{u}} = \mathbf{f} + (\lambda + 2\mu)\nabla(\nabla \cdot \mathbf{u}) - \mu\nabla \times (\nabla \times \mathbf{u}) \quad (3.8)$$

where

- ρ is the density
- $\mathbf{f}$ is the source function (driving force)
- $\mathbf{u}$ is the displacement vector
- λ and μ are the elastic moduli for the solid given by [61]

$$\lambda = \frac{\sigma E}{(1 + \sigma)(1 - 2\sigma)} \quad (3.9)$$

$$\mu = \frac{E}{2(1 + \sigma)} \quad (3.10)$$

Here E and σ are proportionality constants that are specific to the material.

Detailed guidelines on setting up a model for modal analysis using NASTRAN in Autodesk Inventor can be found elsewhere [62], [63].

3.4.1 Vibrational Mode Testing

Once the simulations were completed and the prototype was chosen for fabrication, a 5-axis CNC mill was used to fabricate all the aluminum and some Macor parts. Then, the parts were assembled, and the piezoelectric coarse motors were connected to a function generator. A sine wave function was applied to the z-motor to test the normal modes of the fabricated head. The amplitude was set to 10 Volts, and the frequency was swept from 0 Hz to 20 kHz. This made the z-motor's piezoelectric stacks vibrate with the

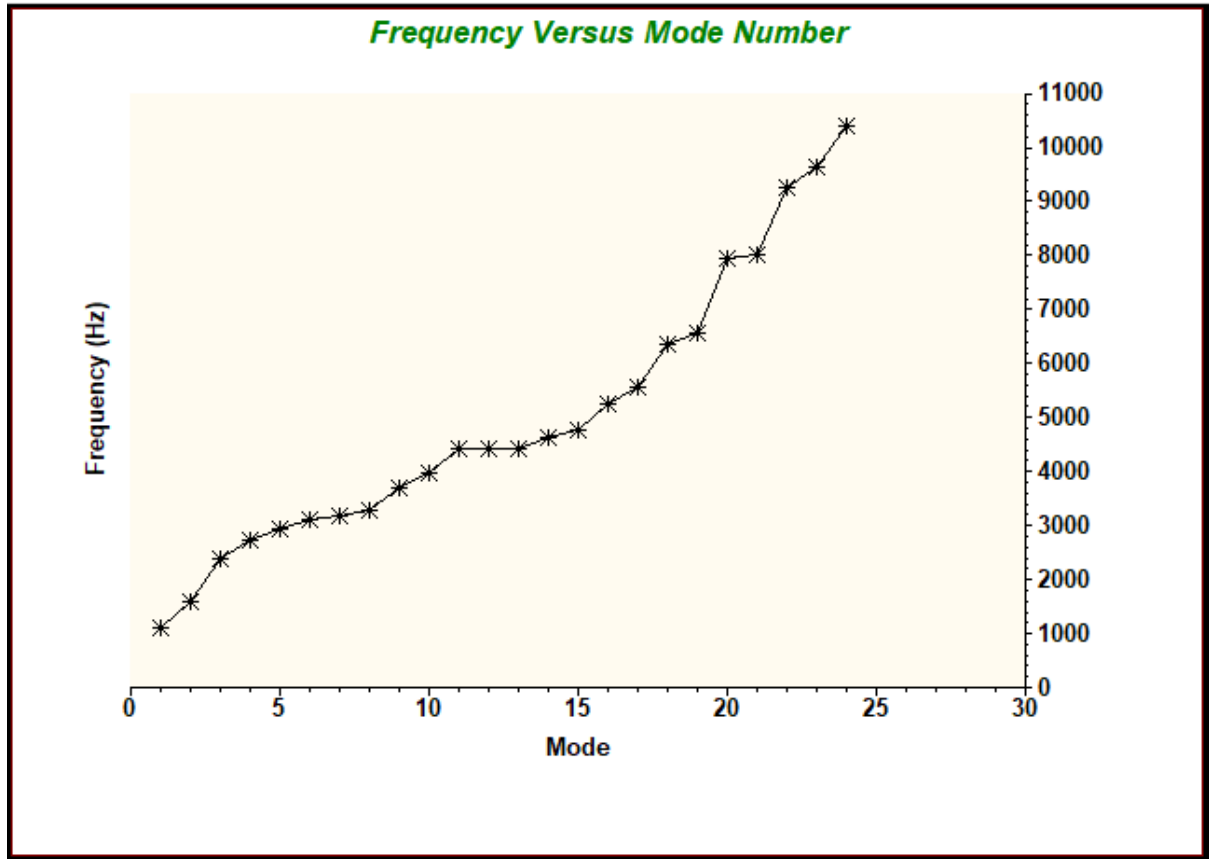


Figure 3.14: Plot of mode number vs the resonant frequency of the current STM head. The lowest normal mode is at 1.12 kHz, and the first 25 modes are shown in the plot.

corresponding frequency, providing an excitation to the entire STM head. Measuring the acoustic response of the STM head as the applied frequency of the sine wave function was changed allowed us to measure the vibrational properties.

The acoustic amplitude was measured using a smartphone application called Spectroid. The data shown in Figure 3.16 is from 6-19 kHz, as the background noise is too high to have accurate acoustic measurements below 6 kHz. The NASTRAN data is shown with orange bars, and the acoustic amplitude measured is shown with a blue line. The peaks of the acoustic amplitudes generally agree with the clusters of the calculated normal modes. This can be seen clearly at around 8 kHz, 11.5 kHz and 15.5 kHz. There will be other, more accurate measurements of the resonant modes done in the future prototypes that are capable of coarse motion, using the STM controller.

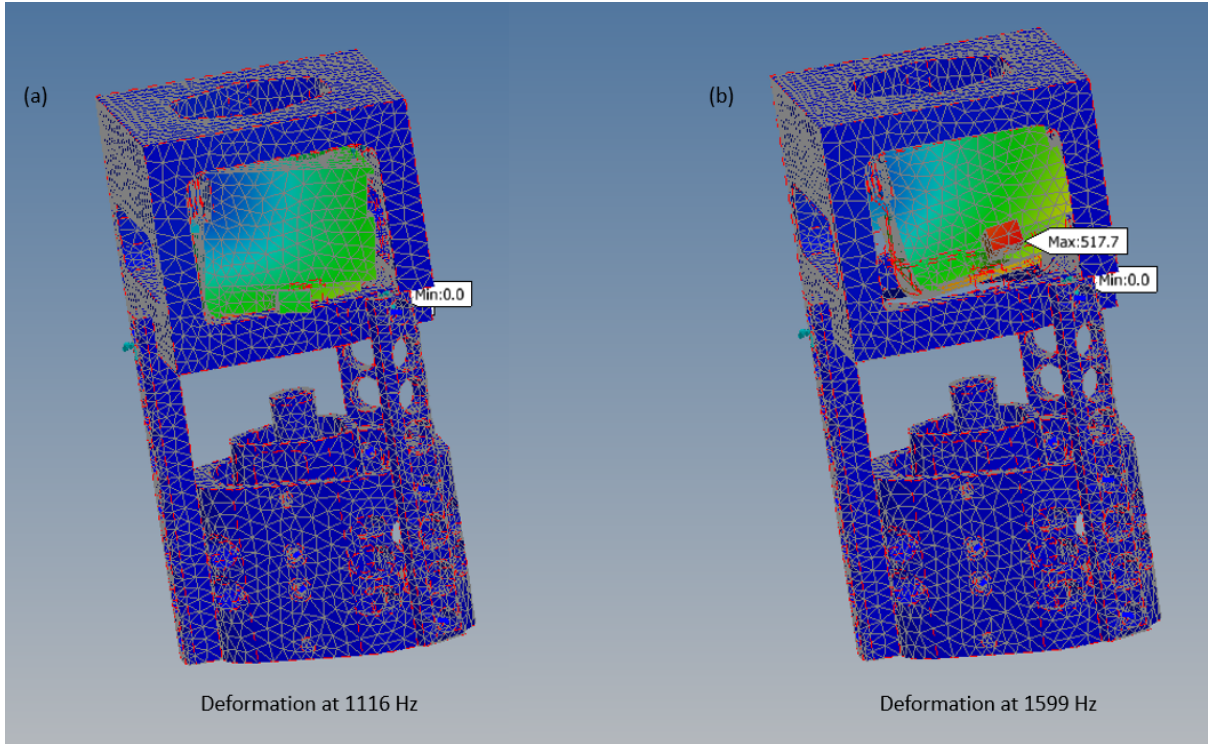


Figure 3.15: Figure showing exaggerated displacement from the first (a) and second (b) normal modes. This can be used to identify the components that contribute the most to these modes, and their designs could be updated to improve the normal mode frequencies.

3.5 Resonant Frequencies

As discussed in the previous sections, the STM head will be suspended with beryllium copper extension springs and placed on an optics table. Since the optics table's pneumatic legs and the beryllium copper springs will filter out all high-frequency vibrations, only low-frequency vibrations will reach the STM head. Therefore, we need the STM head to have high resonant modes to mismatch with the low-frequency vibrations that pass through the vibration filters and remain vibrationally stable for scanning.

The low-frequency vibrations that pass through are below ~ 10 Hz [64], and from NASTRAN analysis, we know that the lowest resonant mode of the STM head is 1.12 kHz, which provides a very large mismatch.

The NASTRAN simulations had to be verified to ensure they were done correctly. This is done in two ways:

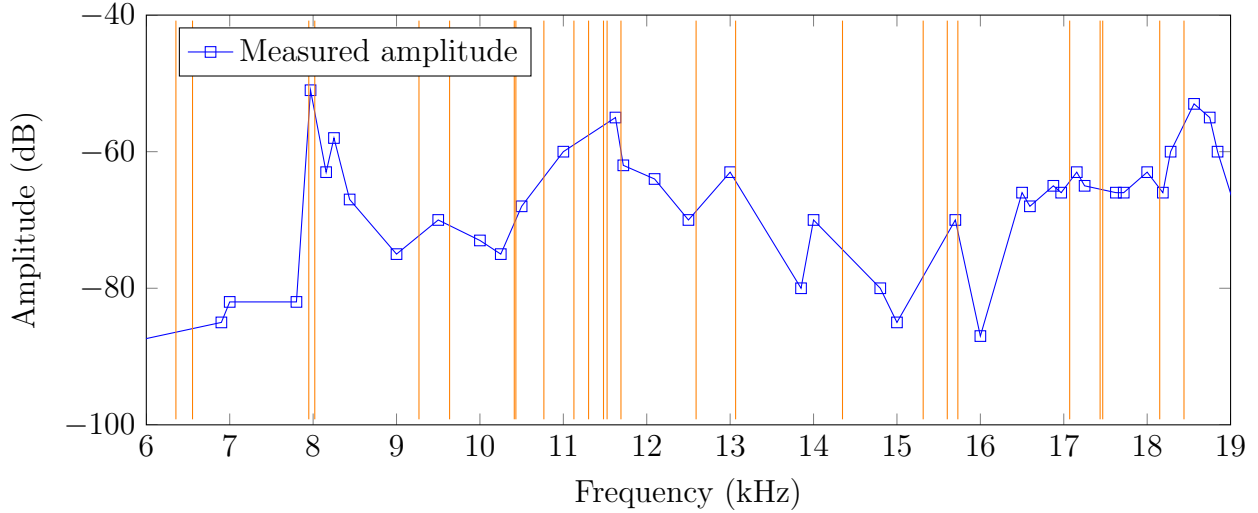


Figure 3.16: The amplitude of resonance measured while applying a sine wave to the STM head. Red vertical lines represent the resonant frequencies calculated from simulations. Amplitudes are negative since zero represents the maximum amplitude the detector can measure. Measurements were started at 6 kHz as the background noise was too high at frequencies below 6 kHz to achieve any useful data.

- First, the output file from the NASTRAN analysis is checked to ensure the “Percent Modal Mass” is above 80%. Physically, this measure gives us the proportion of the mass moving compared to the total mass in the rigid body. Therefore, as long as more than 80% of the mass is moving, the result can be counted as accurate [65]. The effective modal mass calculation in NASTRAN can also be improved by increasing the number of modes considered in the analysis and reducing the size of the individual elements in FEA. However, these changes come at the cost of increased computing power and time required for the simulations to run. Therefore, a balance had to be found, and the goal was kept above 85% “Percent Modal Mass” in each degree of freedom for the STM head. This is higher than the recommended goal from Autodesk, which is above 80%. Table 3.1 shows the Percent Modal Mass obtained from the normal mode analysis of the STM head. Here, the first 150 normal modes were considered, and the directions mentioned in the percent modal mass refer to the three translational and the three rotational degrees of freedom.
- The second way to verify the normal mode calculations was done by applying a sine wave function to the piezoelectric stacks in the z-motor of the STM head.

This allowed the piezoelectric stacks to vibrate with a set frequency that could be controlled by the function generator used to generate the sine wave function as explained in the previous section. The results of this test are shown in Figure 3.16. We can see that most of the peaks align with the calculated resonant mode clusters (especially around 8 kHz, 11.5 kHz, and 15.5 kHz). This further proves the validity of the normal modes calculated for the current STM head design and provides strong evidence that the target for the high resonant frequencies was met.

DIRECTION	TOTAL (kgm ²)	MODAL (kgm ²)	PERCENT
1	1.12e-04	9.82e-05	87.6726
2	1.12e-04	9.66e-05	86.1993
3	1.12e-04	9.55e-05	85.2709
4	1.95e-01	1.75e-01	89.4693
5	6.10e-02	5.29e-02	86.7452
6	1.86e-01	1.67e-01	89.9401

Table 3.1: Output from the normal mode the NASTRAN analysis that shows the Percent Modal Mass from the first 150 normal mode calculations.

There are still resonant modes that do not align with any of the peaks in the acoustic amplitude measurements. This could be because the measurements were done with the STM head, not vertically suspended, compared to the simulations where it was assumed to be vertical. Also, the coaxial wires connected to the piezoelectric stacks were not modelled in the simulations, which could have affected the normal modes calculations of the STM head.

Another difference between the STM head model used in the NASTRAN simulations and the actual STM head was the imperfections from machining. Although the Pocket NC mill is a precise machine for milling softer materials, the rigidity of the mill is lower than a typically large-scale mill for machining aluminum, which produces a lot of vibrations during the fabrication process. This, in turn, caused the fabricated parts to have a poor surface finish, and some chips cut off the surface of larger parts, like the prism cage. Therefore, the final dimensions of the fabricated parts were not the same as the design, which could have altered their normal modes. One positive thing that could

be noted from Figure 3.16 is that the normal modes (~ 6.5 kHz) at the lowest measured frequencies seem to have minimal effect on the STM head, which is the preferred outcome. This will be further validated using the STM controller once the coarse walking stage is redesigned.

Chapter 4

Prototyping and Fabrication

All prototyping and fabrication for this project were done at the Faculty of Science Makerspace and the Physics Machine Shop. Most of the initial prototyping was done using additive manufacturing techniques with plastic printers, and the finalized prototypes were then fabricated with a 5-axis CNC mill out of aluminum for further testing.

4.1 Additive Manufacturing

3D printing (additive manufacturing) fabricates a CAD model using a computer-controlled device to layer material in thin layers until the model is completed. This process is fast and very cost-effective for producing prototypes. Therefore, the STM head design was put through multiple design-prototyping cycles using the rapid prototyping infrastructure in the Faculty of Science 3D maker space. 3D printing is also much faster than conventional fabrication methods, such as subtractive manufacturing, which saves us time, allows us to refine the design more efficiently, and makes the designs more sophisticated.

All additive manufacturing was done using the Original Prusa i3 MK3/MK3s printers. These are Fused Deposition Modelling (FDM) printers that use filaments of thermoplastic materials to fabricate parts [66]. All the prototypes were printed using Polylactic Acid (PLA), a bioplastic most commonly used for 3D printing [67], or Polycarbonate (PC) for when the prototypes require more strength and higher heat tolerance.

These components were assembled with dummy piezoelectric stacks and tube scanners to test for their functionality and design flaws. The components were ready to be machined once the compatibility issues and the design flaws were fixed.

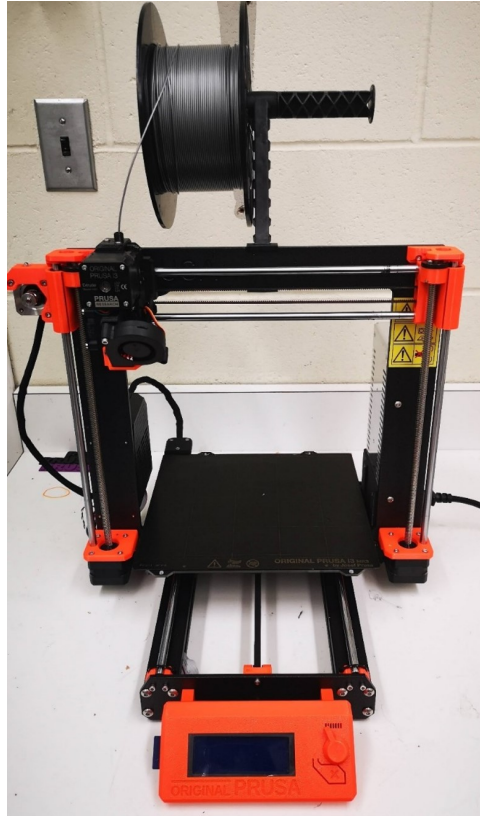


Figure 4.1: A picture of one of the Prusa MK3s printers that were used to make the initial prototypes.

4.2 Subtractive Manufacturing

Once the designs were finalized, the final parts were milled out of aluminum 6061. The primary apparatus used for subtractive manufacturing was a 5-axis CNC mill. Computer Numerical Control (CNC) milling is a type of fabrication that is controlled by computer code. A milling machine uses a rotary cutter to remove material from stock to obtain the required features. It is one of the most common processes used when precision is needed. A milling machine can employ a wide range of tools depending on the feature that needs to be fabricated, but for this project, the largest end mill that could be used in the pocket NC was 1/4 inch. Therefore, all the rough cutting was done using a 6

mm roughing tungsten carbide end mill. Once rough cutting was done, a 6 mm finishing end mill was used to do the last finishing passes on the outer surfaces of the parts. For making the features that were too small for the 6 mm end mill, there was a combination of smaller end mills ranging from 1/8 to 0.031 inch end mills used.

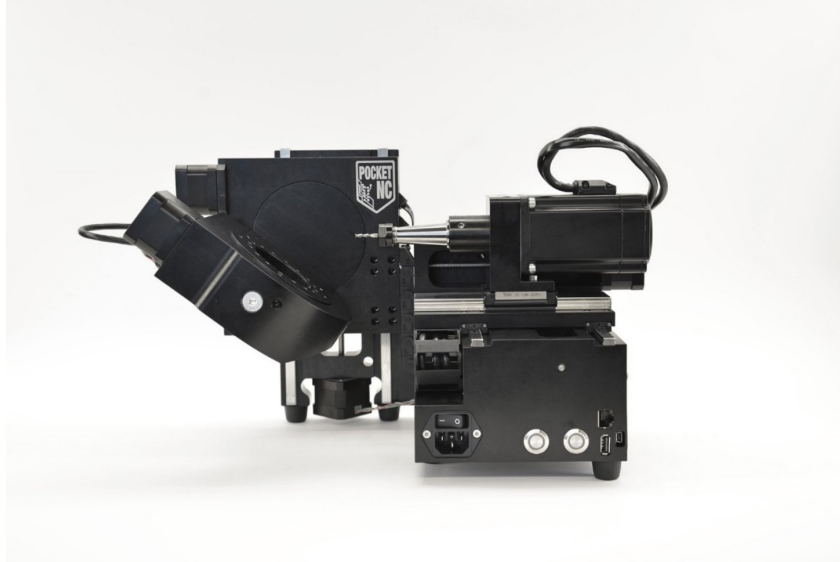


Figure 4.2: Picture of PocketNC V2-10 5-axis CNC mill that was used to make all the aluminum parts in the STM head [68].

The primary machine used for this project was the Pocket NC V2-10 five-axis CNC mill. Although the build volume of this machine is small (5.0 inches/128.3 mm (Y), 4.55 inches/115.5mm (X) and 3.55 inches/90.1mm (Z)), the easy accessibility to tools and the simple architecture of the machine made it ideal for the fabrication of parts for this project. Also, all the parts of the STM head were designed to fit in the machine's footprint, as this was the only CNC mill available at the beginning of this project. The end mills used for this project were all made of tungsten carbide, and most of the bulk clearing of material was done with a six-millimetre four-flute end mill to save time. Finishing passes and the smaller features were made using smaller end mills or end mills with more flutes. The speeds and feed rates used for milling the components are provided in Appendix B. MACOR was one of the most challenging materials to mill because of its hardness and tendency to shatter. Machining must be done extremely slowly with a rigid mount. Due to these machining problems, the design of the STM head was altered to use as many pre-made MACOR parts as possible. The speeds and feed rates for machining MACOR ceramics are also provided in Appendix B.

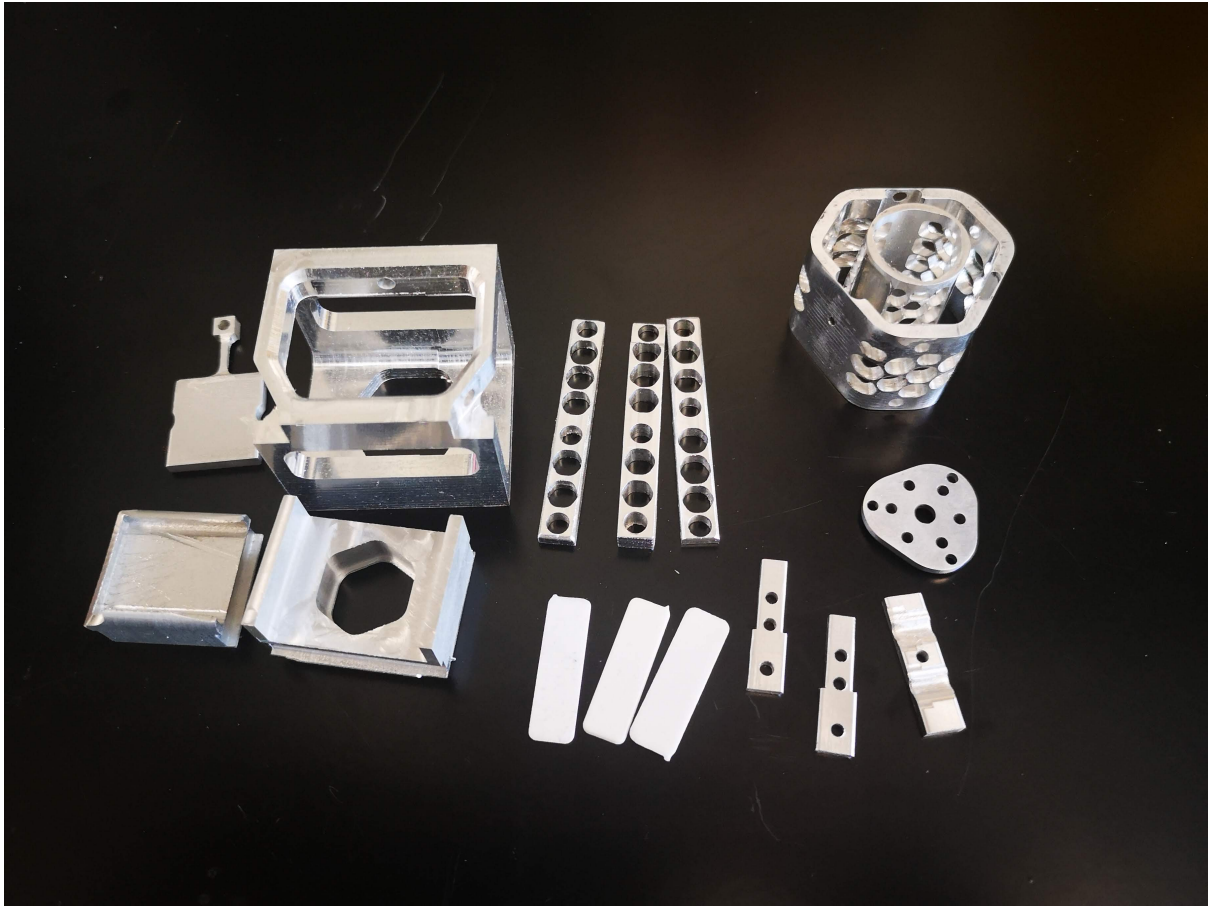


Figure 4.3: All the STM head components that were machined out of aluminum using the PocketNC CNC mill.

4.2.1 Machining Limitations

Subtractive manufacturing is ideal for making more robust and rigid parts, but this process has many limitations regarding complex designs and reducing mass. This is because of the nature of removing material with a tool in subtractive manufacturing. Since all the work is done with a tool, features accessible by the tool are the only ones that could be made. Some features that cannot be made with conventional subtractive manufacturing are hollow pockets with no openings (or narrow openings) and pockets with square edges.

The STM head design had to be altered multiple times from the original prototypes made with 3D printing to be compatible with the 5-axis mill and the tools available for the project. One of the major features that had to be redesigned was the slots in the prism cage for the cage inserts. The slots have a dovetail cut designed to be machined

with a 0.062-inch end mill. However, the slots were too deep (22 mm), and no available end mills could machine them. The design had to be changed so that the dovetail cuts only reached the point accessible to the end mill (9mm), as shown in Figure 4.4. Some other problems faced during the transition from additive to subtractive manufacturing during the prototyping process were overcome by finishing the parts on a manual mill for features that could not be milled with the CNC mill. One of the features that was done this way was the screw holes in the prism. Due to the shape of the prism, the optimal way to mill it was upside down in the CNC mill, so the screw holes were not machined until after it was removed from the CNC mill. This affected the precision of the location of the screw holes in the prism.

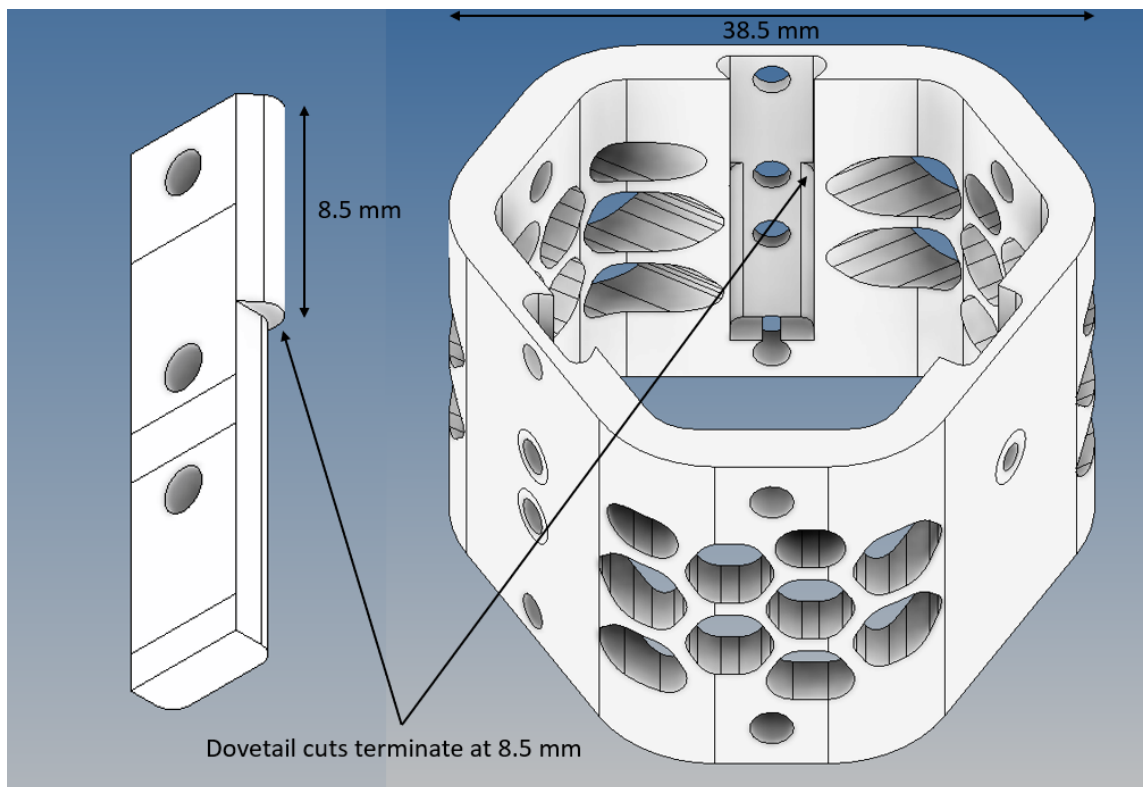


Figure 4.4: Dovetail slots and inserts with the updated design.

4.3 Metal 3D Printing

During the last year of this project, a metal 3D printer was purchased for the Faculty of Science Maker Space. The printer, TRUMPF TruPrint 1000, is an SLM (Selective Laser Melting) machine that uses a laser to melt metal powder layer by layer to make the

part from a CAD model. This machine eliminates almost all the design constraints that subtractive manufacturing brings while preserving the strength and rigidity of the parts. It also allows us to use harder and stronger materials, such as Titanium and Tungsten, than the aluminum used for the STM head in this project. The next prototype of the STM head is currently being built with this printer, and the material choice for that version is titanium, as it complies with all the material requirements for the STM head.



Figure 4.5: TRUMPF TruPrint 1000, the printer used for all additive manufacturing of metals in this project.

Subtractive manufacturing is also limited by the size of the tools available, which determines the size of the features in a part. Meanwhile, with additive manufacturing,

the feature size is only limited by the laser focal point diameter, powder grain size and layer height, which are measured on micrometre scales. This allows the STM head part to shrink in size, have smaller and thinner features (because of the capability of making smaller features as well as the use of stronger metals) and have better rigidity since having a much more complicated design would not have much of an effect on the fabrication time.

Printing with this machine involves a high-power laser, metal powder and an inert environment to prevent the metal powder from combusting. Some metal powders (Titanium) are more combustible and require inertization before printing. This is done by filling the build chamber with argon gas so that there is no oxygen for the powder to react with while the laser melts the powder. The printer has a laser focus point diameter of $54\text{ }\mu\text{m}$, hence x/y precision of $54\text{ }\mu\text{m}$. The minimum layer height is $10\text{ }\mu\text{m}$. Thus, the z-axis precision is $10\text{ }\mu\text{m}$. The printer lays a thin layer of powder (~ 20 microns thick) on top of the build surface, and the laser melts this powder into the shape determined by the CAD model. This process is repeated until the whole part is built. The part requires supports for any overhangs, as well as supports at the bottom so that it can be removed from the build plate.

4.3.1 Titanium

The primary material for the next prototype of the STM head will be switched from aluminum to titanium. Titanium offers various advantages over aluminum, such as a higher hardness scale, higher tensile strength, and better rigidity. This allows the parts to have much thinner walls, and since titanium is also non-magnetic, it is the ideal material for the STM head.

The TRUMF TruPrint 1000 can print grade 5 titanium using the Ti-6Al-4V titanium alloy powder. This powder is highly precise, with a low oxygen content, high density (bulk and tapped), and a controlled grain size [69]. The design for the first prototype of the Ti STM head was an altered version of the Al STM head. The main difference is in the prism cage, where an additional part controls the spring force applied to the prism, as shown in Figure 4.6. This prototype is derived from a design made for subtractive manufacturing with the constraints of milling. However, a new original STM

head design needs to be created to take advantage of all the capabilities that additive manufacturing offers.

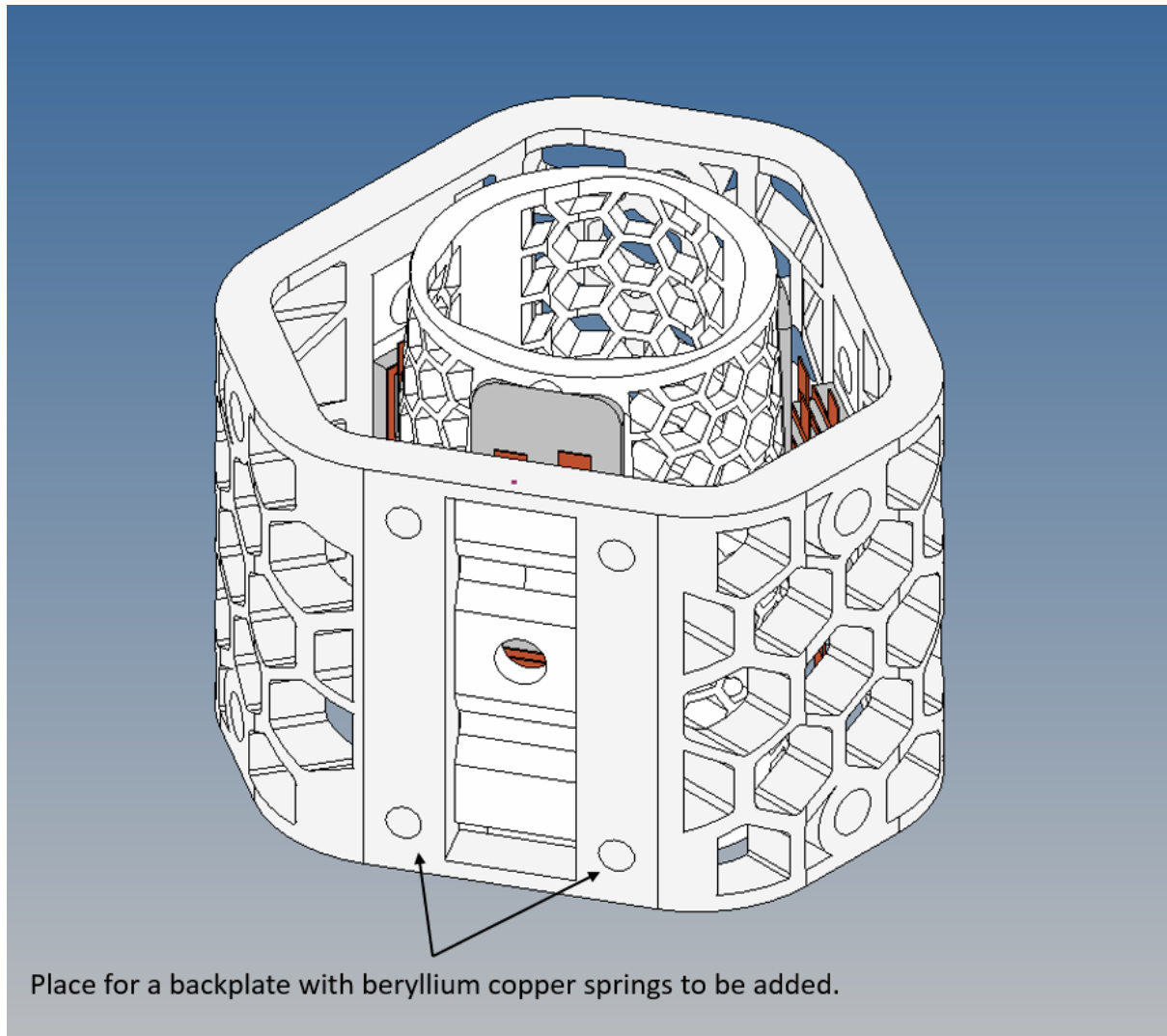


Figure 4.6: Updated design for additive manufacturing with adjustable spring force applied through an extra back plate where the beryllium copper leaf springs will be attached. The screws securing the back plate will have additional compression springs to fine-tune the spring force applied to the piezoelectric stacks.

4.3.2 Tungsten

One of the samples that is of interest for the STM experiments is tungsten with thin layers of iron (Fe) grown on it. However, to prepare the tungsten sample for the STM, it must be baked at around 2000° Celsius. This poses a big problem since most materials

have a melting point lower than 2000° Celsius and thus cannot be used to make a sample preparation stage. Therefore, we created the sample preparation stage using tungsten to withstand the temperature. However, machining tungsten is challenging because of its hardness and brittle nature, so 3D printing with tungsten was the ideal choice.

After some test prints and adjustments to the print settings, the TRUMPF TruPrint 1000 was able to print Tekna spherical tungsten powder. However, the printed parts were very brittle and had to be handled with care. The initial prints also suffered from oxidization while being printed, which affected the layer adhesion in the parts and made the parts weaker. The oxygen level in the chamber had to be brought down from the recommended 0.3% to 100 ppm to avoid oxidization while printing. The amount of powder carried by the recoater was also increased by 300% to improve the spread of the tungsten powder. This was probably due to the higher density and mass of the tungsten powder.

The design for the sample heating stage is shown in Figure 4.7. The print settings for Tekna spherical tungsten powder are available in Appendix D.

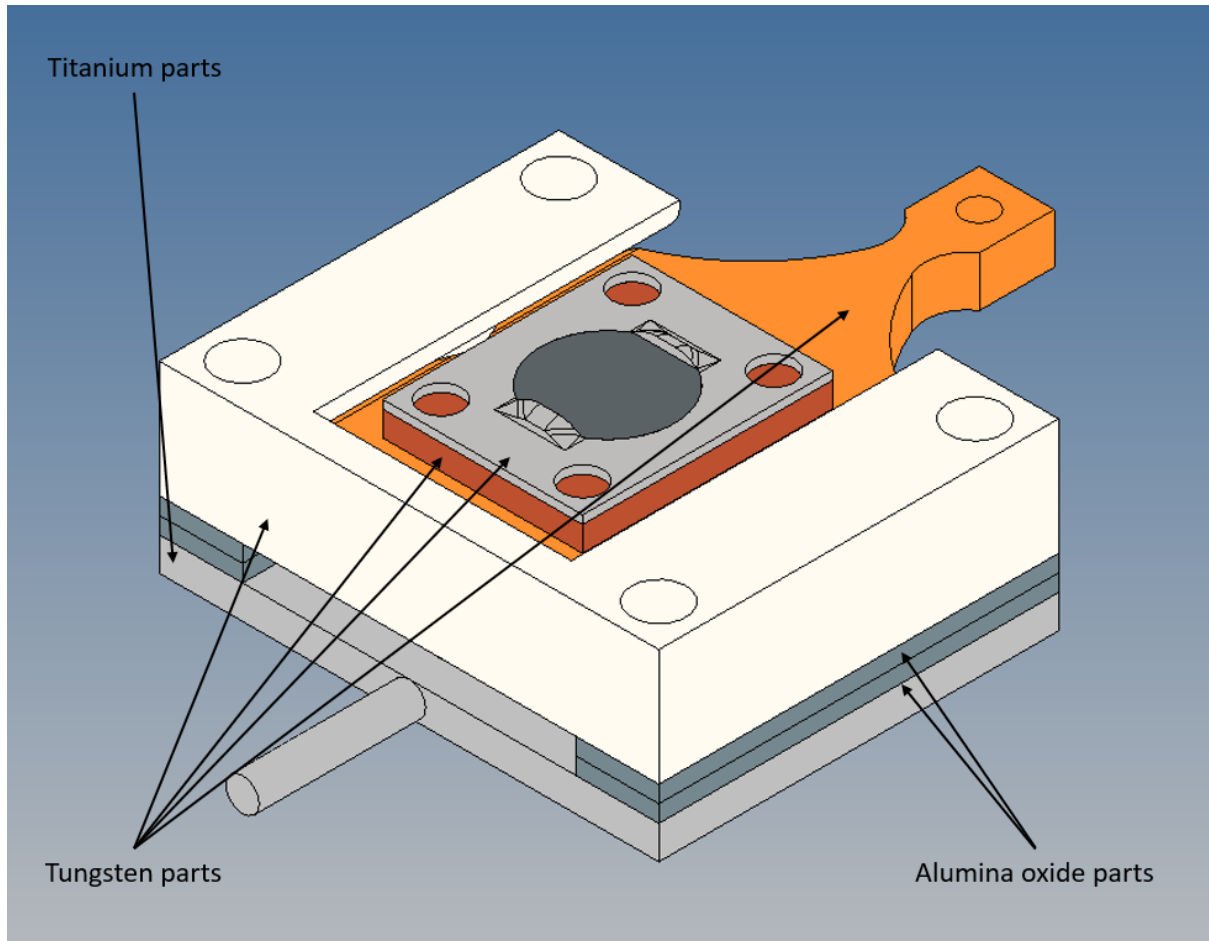


Figure 4.7: One of the prep chamber stages used to prepare tungsten samples by heating them to about 2000° Celsius to prepare them for scanning. All the parts that are immediately next to the tungsten sample are made of tungsten as well so that they can withstand high temperatures and help radiate the heat away. There are Alumina oxide parts after this to provide a heat barrier between the tungsten and the titanium parts.

Chapter 5

Assembly and Testing

The assembly and testing of components for the STM was one of this project's most crucial and tedious parts. Once all the parts were fabricated, they were prepared for their respective assembly process. This chapter discusses the assembly process for the piezoelectric stacks, the final STM head assembly and the UHV chamber assembly.

5.1 Piezoelectric Stacks

Piezoelectric ceramics control all motion in the STM head. As discussed in previous chapters, the piezoelectric tube controls all fine motions, and piezoelectric slabs control all coarse motions. The piezoelectric materials used for this project were EBL #2 (PZT-5A), EBL #3 (PZT-5H) piezoelectric shear plates and EBL #2 (PZT-5A) tubes acquired from EBL Products Inc. The datasheets for the piezoelectric materials can be found on their website [67]. The piezoelectric slabs used for coarse motion cannot individually move the prism in large enough steps. Therefore, we stack them to make piezoelectric stacks that can achieve the required step size. Each stack contains three EBL #2 piezoelectric slabs for extended motion sandwiched between copper plates, as shown in Figure 5.2. This provides control over individual piezoelectric slabs in each stack for testing and reduces step size when required.

As shown in Figure 5.2, each piezoelectric stack contains three shear plate piezos,

four copper plates, an alumina oxide plate and a sapphire crystal. The role of the alumina oxide plate is to act as an electrical insulating barrier between the copper plates and the cage insert to which the stacks are going to be attached. This prevents the stacks from electrically shorting with the other stacks via the prism cage. The anatomy of the piezoelectric stacks starts with the alumina oxide plate attached to a copper plate. Then, there are three alternating shear plate piezos and copper plates sandwiched on top of each other, and finally, a sapphire crystal is glued on top of the last copper plate.

Appendix C provides detailed instructions on assembling the piezoelectric stacks. One of the most important things to consider when constructing the stacks is the polarization orientation of the piezoelectric slabs. The piezoelectric slab deforms in one direction as a voltage difference is applied across it, and the stacks need to be oriented as shown in Figure 5.1 so that the motion of the slabs does not cancel. In this Figure, the arrows indicate the direction of deformation for the piezoelectric slabs. Initial stacks were made of nickel-plated piezoelectric slabs to test the assembly process, as they were not compliant with the STM head's requirements. Once the assembly process was shown to work, the nickel-plated piezoelectric slabs were replaced with gold-plated slabs so that the stacks were non-magnetic. The test stacks made with nickel-plated slabs also helped study the conductivity of the EPO-TEK H21D epoxy used to assemble the stacks. The epoxy did not have the required conductivity for the stacks to perform optimally, and extra care had to be taken while gluing so that the copper plates made direct contact with the piezoelectric slabs instead of the epoxy making an insulating layer. This was done by constantly checking the conductivity between the gold on the piezoelectric slabs and the copper plates during the gluing process. The epoxy also adds to the thickness of the piezoelectric stacks. This was not initially considered for simulations and CAD assembly, but it had to be taken into consideration later. This height change in the stacks was not identical; the stacks with similar heights were paired up during the STM head assembly process. The heights of the stacks after assembly are shown in Table 5.1.

Once the stacks were assembled and glued, the coaxial wires were added to the copper plates. This was done using the same conductive epoxy initially. However, once the conductivity problem was discovered, the epoxy was replaced with spot welding the wires onto the copper plates. Some copper plates had tabs that were not ideal for spot

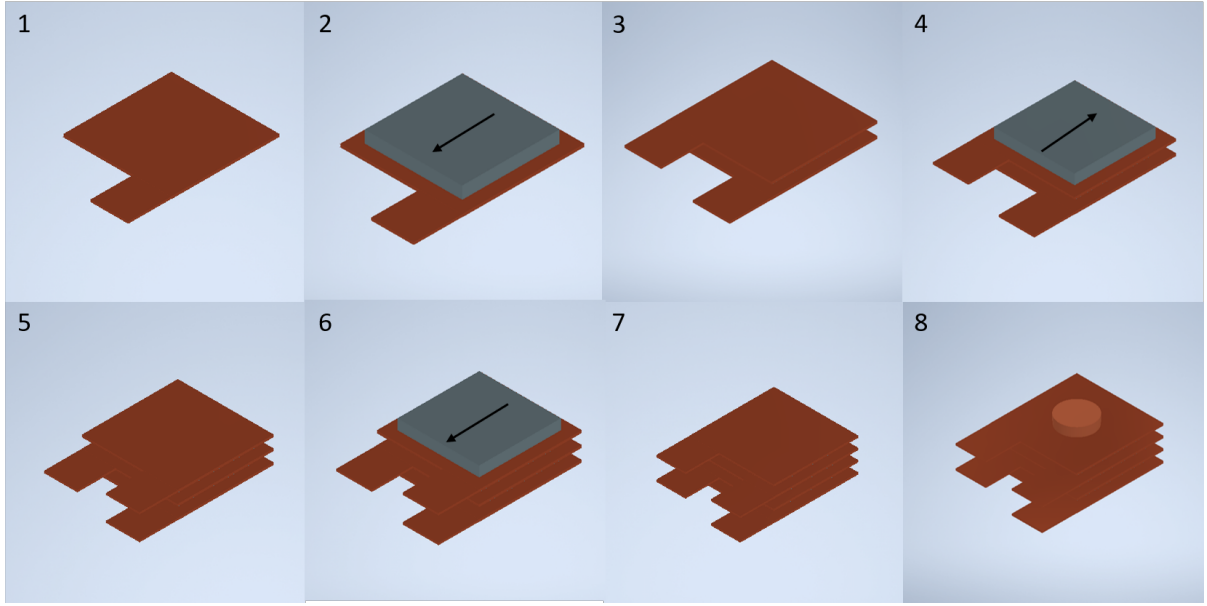


Figure 5.1: Order and orientation in which the piezoelectric stacks were assembled and glued.

Stack Number	Height (mm) $\pm 0.02\text{mm}$
1	3.66
2	3.64
3	3.70
4	3.57
5	3.54
6	3.72

Table 5.1: Thickness of the assembled piezoelectric stacks.

welding, and in those cases, the wires were soldered using EutecRod 157 UHV-compatible solder. Kapton insulated silver-plated copper wires were used for all the wiring since they are also UHV compatible. During the soldering and spot-welding processes, extra care had to be taken so that the piezoelectric slabs did not heat too much and get depolarized. Spot welding was the preferred process since spot welding applies less heat than soldering, and soldering adds extra material, increasing the mass of the piezoelectric stacks, which is not ideal [70].

Each piezoelectric stack is topped off with a sapphire crystal to reduce wear from the stick-slip motion. Since conductivity is unnecessary here, these sapphire crystals

are glued on using EPO-TEK H74 UHV-compatible epoxy. The wires attached to the piezoelectric stacks were about 10 cm long, as this would prevent the wires from getting tangled and help identify the wires' polarity easily. At the other end of these wires, pin and sleeve connectors were added so that the wires could be attached to the wires from the STM controller.

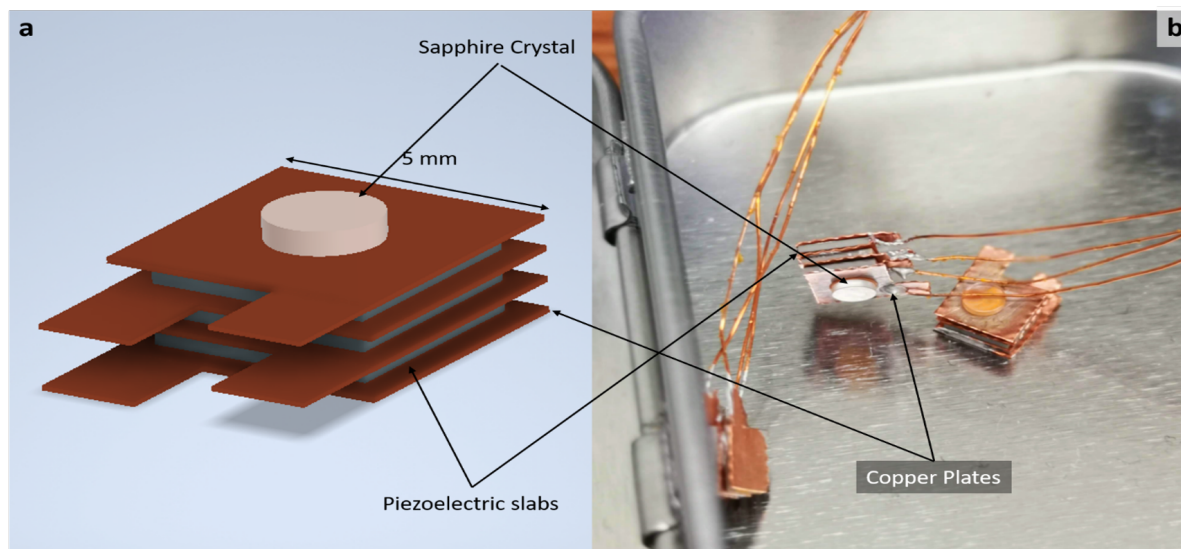


Figure 5.2: Shear plate piezoelectric stacks assembled, glued and baked.

5.2 STM Head Assembly

Once the piezoelectric stacks were assembled, they were glued to the prism cage inserts with the copper plate facing outwards, as shown in Figure 5.3. At this point, the STM head is ready for the final assembly procedure. This was a tedious process as the thin wires from the piezoelectric stacks got tangled during the assembly process. One of the major troubles during the final assembly process was the piezoelectric stack wires detaching from the copper plates if they got caught on anything during the assembly process. If this happens, the head must be taken apart for the wire to be attached back on. After many accidents with the wire detaching, the assembly procedure was changed, where the wire's other end would be connected to breadboards using the pin connectors to keep the wires steady during the assembly process. This made the assembly manageable, and the head was assembled, as shown in Figure 5.4.

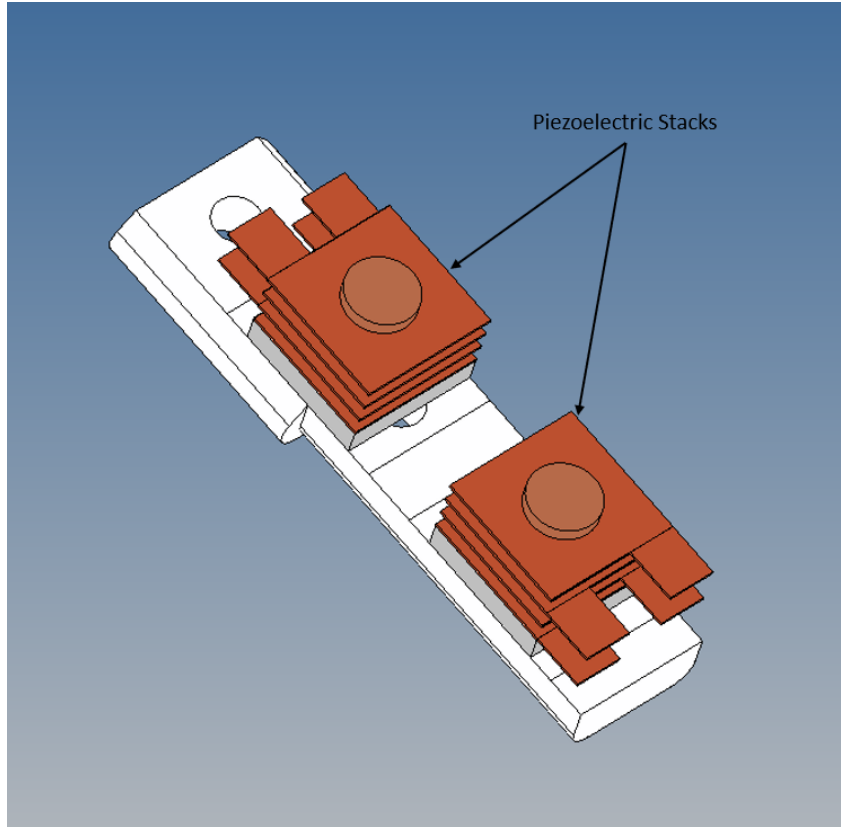


Figure 5.3: Piezoelectric stacks glued facing away from each other for easier wiring of the stacks.

Once the STM head is transferred to the UHV chamber, there will be pre-assembled wires in the chamber with socket connectors for the piezoelectric stack wires to attach to. This should make the wiring in the chamber more manageable as the longer wires will be installed before the STM head. A PEEK holder will be used in UHV to replace the breadboard and make the wiring manageable as well.

The final assembly process for the scan head is aligning the prism and the three prism cage inserts, as shown in Figure 5.4, and inserting them carefully into the prism cage. This was a tight fit, and since the piezoelectric stacks were not all the same height, the tension force applied was not the same as expected during the design and simulation process. This could also be the reason for the discrete tension system for the prism failing. This is an unavoidable problem since the thickness of the epoxy used in the piezoelectric stacks can easily vary between layers. The additive-manufactured STM head that supersedes the current design can avoid this problem by using a continuously

adjustable spring tension design.

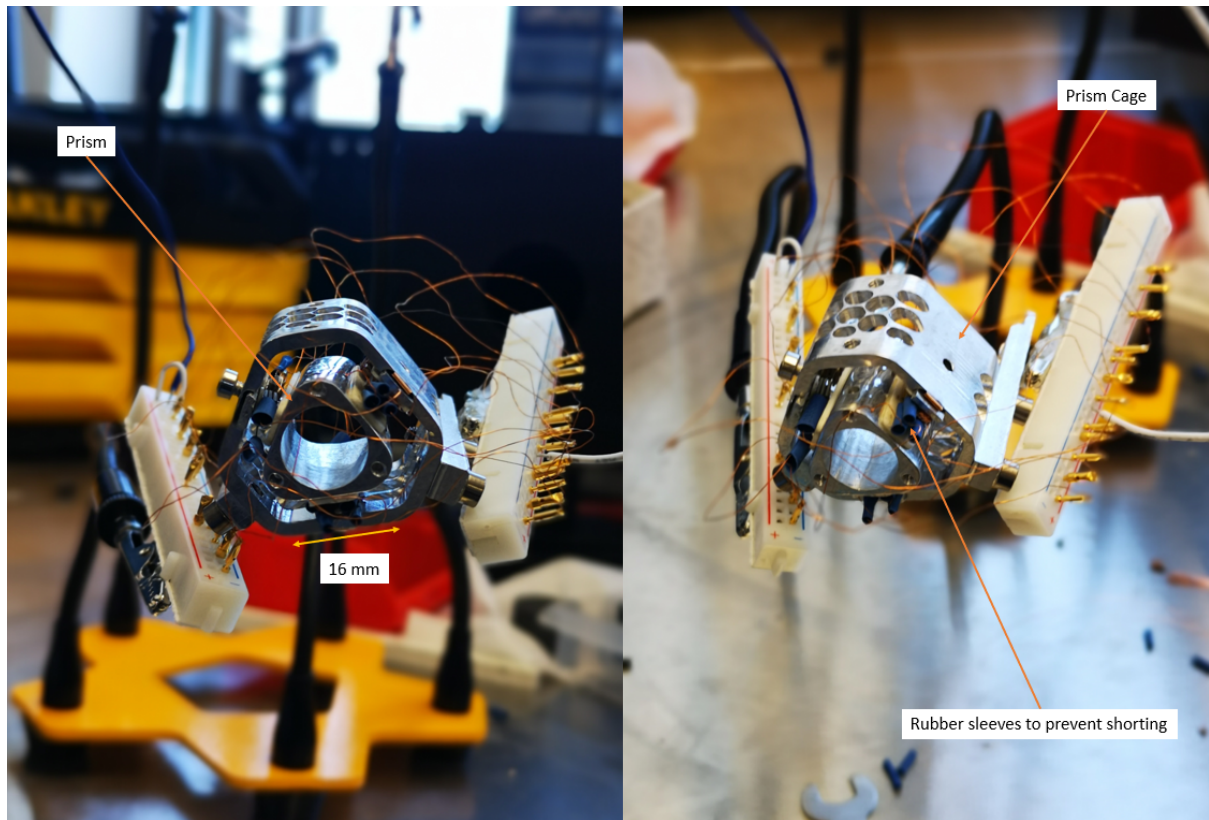


Figure 5.4: Prism inserted into the prism cage and being held by the piezoelectric stacks and the beryllium copper springs. The piezoelectric stack wires are connected to breadboards for testing coarse walking.

The necessary steps for final assembly are:

- First, all the components are sonicated in acetone to remove all the foreign particles and dust. Then, the parts are sonicated in methanol to remove all the acetone.
- Once the parts are clean, the non-conductive epoxy is prepared and applied to the beryllium copper springs and the prism inserts. The springs and the prism inserts are placed in their designated spots in the prism cage and the prism, respectively, and baked at 100° Celsius for 20 minutes for the epoxy to cure.
- After the parts are baked, they are allowed to cool down. Then, the prism cage is attached to a clamping arm with two breadboards around it.

- The piezoelectric stacks are then brought in, and their wires are connected to the breadboards so that they don't get tangled, and the polarity of the wires can be easily identified.
- Then, the prism is brought in and placed in the middle of the three prism cage inserts, and they are all lowered into the cage simultaneously. This is the best way for the final assembly, as the prism is a tight fit inside the cage.
- Once the dove-tail cage inserts are in their designated slots, the titanium screws are added to the cage inserts through the cage, as shown in Figure 5.4, to fix them in their place and provide better rigidity.
- Finally, one last screw is added to the last cage insert to prevent any lateral movements and only allow the insert to be pushed in one direction by the beryllium copper leaf springs.

Once the assembly procedure was completed, the coarse walking stage was tested by applying a sine wave function to ensure each piezoelectric stack was functioning. This was done by changing the frequency of the sine wave function and measuring the acoustic amplitude using a smartphone application to check if the acoustic amplitude peak matches the applied frequency. The results of this test are shown in Chapter 3. Once the piezoelectric stacks were shown to be functional, coarse walking was tested using a saw tooth wave pattern provided by the coarse walking stage controller built in the lab by Dr. Burgess. Initial tests showed that the piezos were working, but no motion of the Prism could be detected. This could be due to the applied spring tension being too much.

The other major problem with the current design was the piezo wires shorting to each other. As the wires are very close to each other at the piezoelectric stacks, when a high voltage is applied, they make a short in the circuit. Rubber sleeves were added to the piezoelectric stack ends of the wire to prevent shorting. However, the sleeves did not work every time, and due to the thinness of the wires, it was difficult to keep them managed properly during the assembly process as well. This could have also affected the coarse walking tests. Another possibility of the Z-motor not being able to move the prism

is that the piezos could have shorted after moving the prism for a short distance. Further evidence of this was seen during one of the tests where the stacks had no shorts initially, but after the prism was allowed to move more shorts appeared. This also suggests that the coarse motor design would work if not for the shorts in the piezoelectric stacks.

Future designs of the STM head could prevent these types of shorting by adding a custom PEEK holder that keeps the piezoelectric wires separated near the piezoelectric stacks. As the PEEK holder would be more rigid and attached to the prism cage inserts, it will not detach during coarse walking, unlike the rubber sleeves.

In conclusion, the two major design goals for the next STM head prototype are to have adjustable spring tension to the prism and have better piezoelectric wire management integrated into the design to prevent shorts.

5.3 UHV Chambers Assembly

The UHV chambers were originally designed by Dr. Burgess and contain a mixture of custom-made and off-the-shelf parts made by Kurt J. Lesker Company [71]. However, some parts of the design had to be redone and rearranged for this project. The primary skeleton of the UHV chamber assembly consists of three main parts: load lock, prep chamber assembly and scan chamber assembly. All the UHV chamber assembly components are connected using ConFlat (CF) fittings to hold the UHV pressure without any leaks to the atmosphere. CF flanges use a combination of a copper gasket and stainless-steel knife edges to make a nearly impenetrable vacuum barrier.

The UHV chamber assembly sits on an aluminum strut frame on the optics table, as shown in Figure 5.8. The aluminum struts were cut and assembled in the lab with the chamber design in mind. Once the primary sections of the frame were constructed, the prep and scan chambers were lowered onto customized holders and bolted in. The next step was to extend the frame towards the load lock region and add the load lock onto the prep chamber. All the ports in the chambers smaller than 4 inches in diameter use 1/4 inch bolts, and the ports 4 inches in diameter or larger use 5/16 bolts to connect.

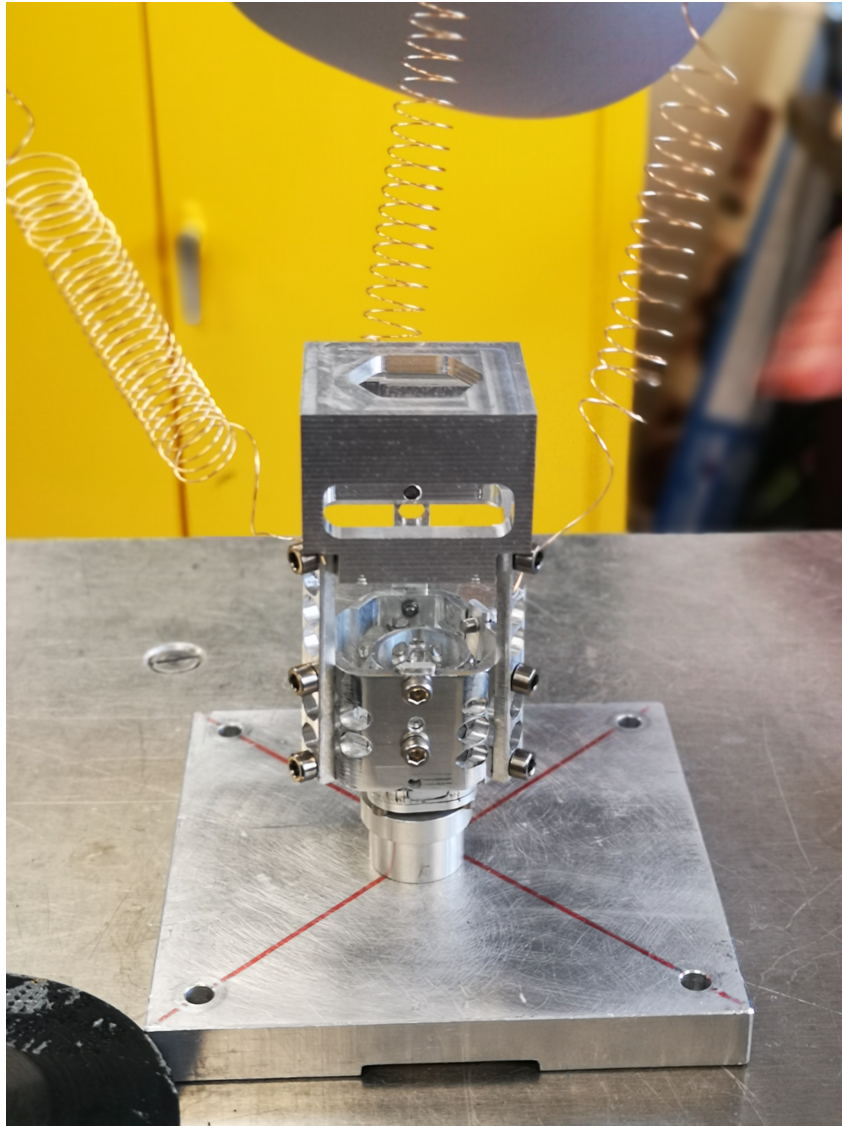


Figure 5.5: STM head assembled and ready for testing.

The rest of the assembly was built in the following order:

- The load lock section of the frame was extended for the turbo pump to be added.
- Two more frame extensions at the prep and scan chambers were added to hold the ion pumps.
- A Residual Gas Analyzer (RGA) was added to the prep chamber.
- Thermocouples and wobble sticks were added to the prep and scan chambers.
- Transfer arms were added to the prep chamber and the load lock.

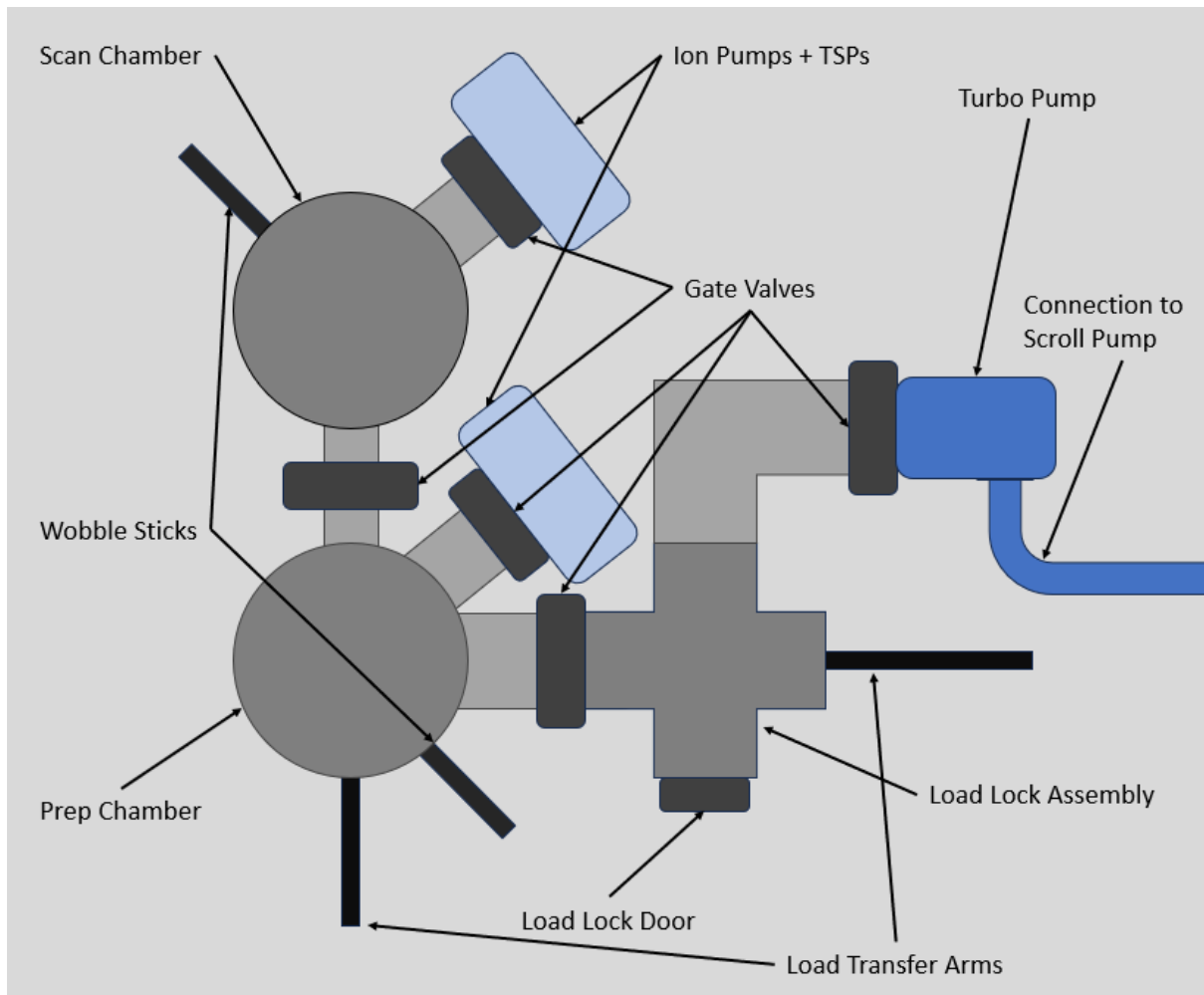


Figure 5.6: Diagram showing the layout of the UHV chambers and their main components.

- Bake-out bulbs were added to both the chambers and the load lock (The bulb in the load lock was too long and had to be bent to fit around the transfer arm).
- Next, all the remaining manipulators and feed-throughs were added to the chambers.
- The ion pumps were added to both chambers.
- Finally, the two z-axis linear shift manipulators were added to the top ports of the prep and scan chambers.
- The cold head, responsible for cooling the STM head, must be lifted in and out of its holder in the scan chamber. Therefore, using aluminum struts, a custom crane was built to hold the cold head in place above the scan chamber.

- The cold head is then attached to the z-axis manipulator on top of the scan chamber, as shown in Figure 5.7.
- Finally, the remaining flanges were covered with windows.

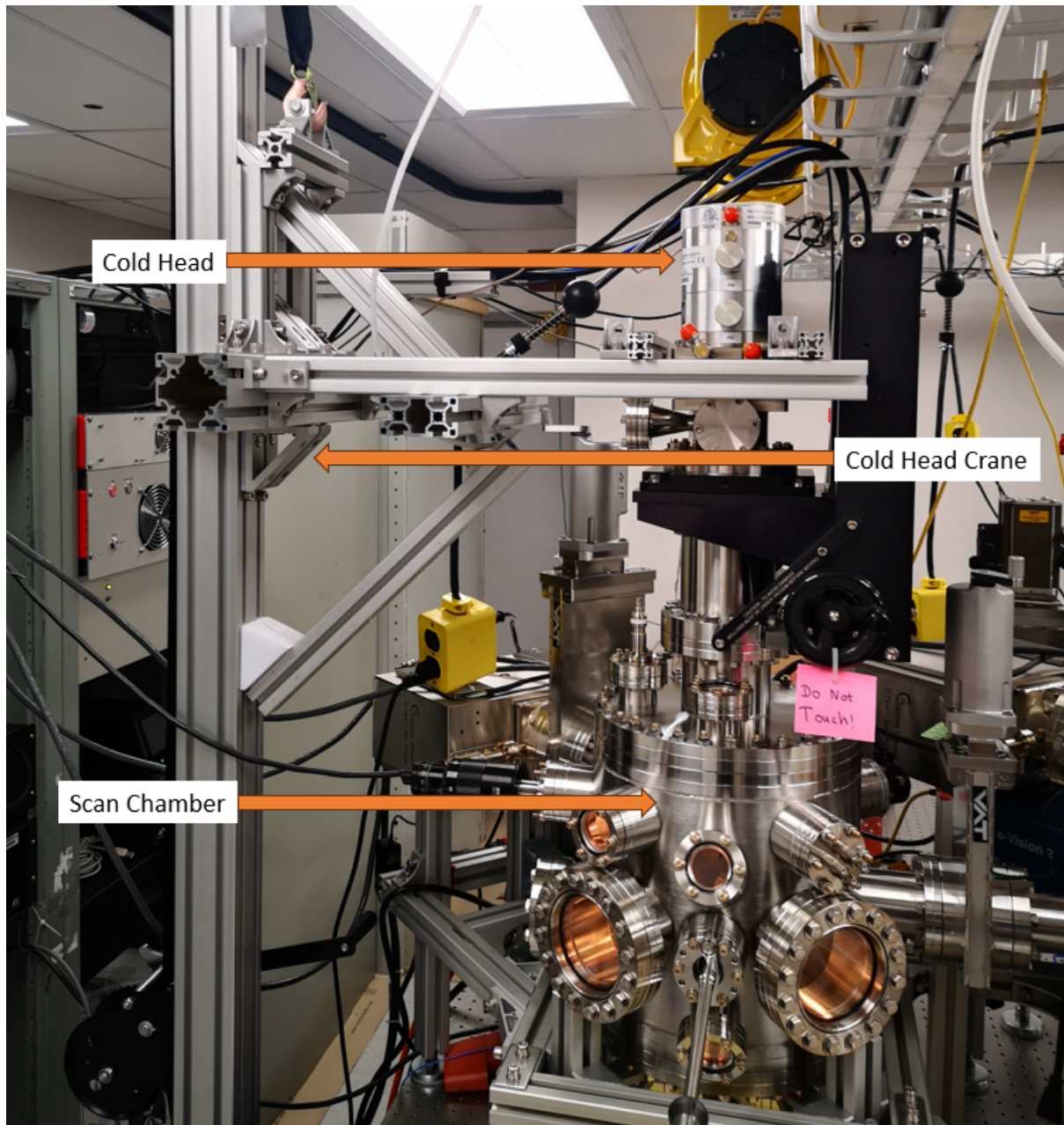


Figure 5.7: Picture of the cold head being held by the cold head crane over the scan chamber.

All these components had CF fittings to be UHV compatible and were connected using 1/4-28 or 5/16 bolts. The bolts were tightened in a clockwise fashion until the

required torque was reached using a torque wrench.

Once the UHV chamber assembly was completed, the chambers were pumped down to high vacuum levels to check for leaks. This was done by initially ensuring all the bolts were tightened to the recommended torque of each flange (the flange size determines the required torques). Then helium gas was sprayed into the flange gaps to see if pressure changed in the chambers. Since helium atoms are small, they could get through any small gaps in the chamber flanges and help identify leaks. Leaks were found in the sapphire windows at the bottom of the scan chamber, which were fixed by removing and reinstalling the windows. The next step was to turn on the ion and TSP pumps to bring the chambers down to UHV levels. The scan chamber reached 10^{-10} Torr, which is excellent for an unbaked UHV chamber. However, the prep chamber did not go below 9×10^{-9} Torr, which leads us to believe there might be a small leak in this chamber that needs further testing.

All three sections of the UHV chamber assembly are isolated from each other using UHV gate valves that are manually controlled, as shown in Figure 5.6. A UHV gate valve allows us to control the flow of gases between these chamber assemblies and is made of a sliding gate that can be moved to either block or allow passage for gasses. These gate valves can effectively seal off the chambers from one another. The gate valves are robustly constructed of stainless steel and provide reliable sealing without any friction at the gate seal [72]. The lubricant-free design allows the gate valve to be baked at up to 250° C to achieve UHV conditions. One last gate valve in the load lock assembly is pneumatically controlled and is used to separate the load lock assembly from the turbo and scroll pumps. This gate valve is powered by the Allen building compressed air supply.

The load lock has a door for the sample tray to be loaded in, and the sample will be transferred to the sample prep stage via the first transfer arm. The sample will be taken off the transfer arm using the wobble stick and transferred to the appropriate prep stage in the prep chamber. Once the sample is prepped for scanning, it will be loaded onto the second transfer arm and moved to the scan chamber. Here, another wobble stick will be used to move the sample tray off the transfer and onto the STM head for scanning. This process allows the chamber to be in UHV while the sample is loaded and helps store multiple samples in the prep chamber for faster scans.

The whole assembly is pumped down to high vacuum levels with the turbo and the scroll pumps, and then the ion and titanium sublimation pumps (TSPs) take over, bringing the chambers down to UHV levels and holding them there. At this point, the gate valve to the turbo pump is closed, and the chamber is sealed from the atmosphere.

This assembly allows the STM to reach its maximum potential and be able to achieve the goals set out at the beginning of this thesis.

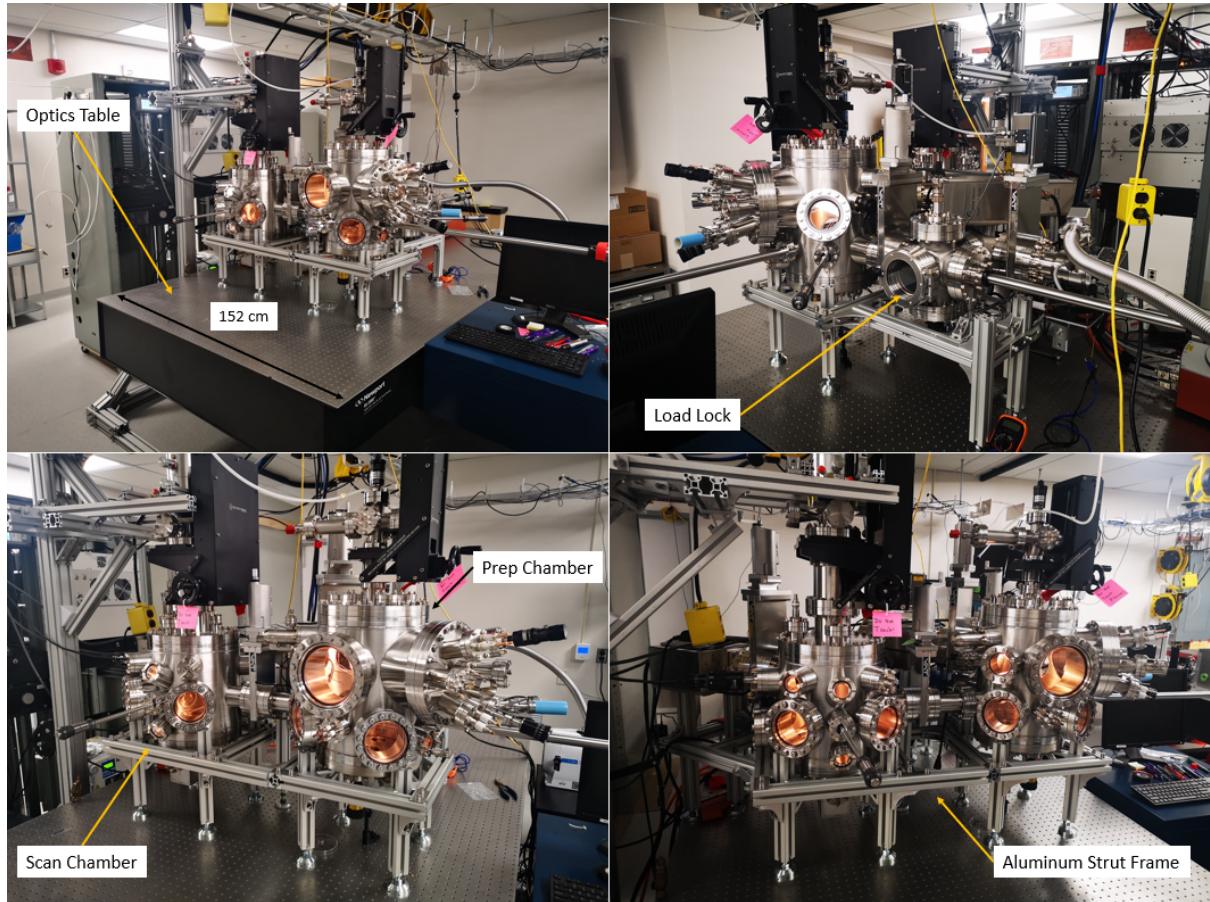


Figure 5.8: Pictures of the assembled UHV chambers and the optics table they sit on.

Chapter 6

Future Work - Titanium STM Head

The design and fabrication of custom STM heads for the Ultrafast Microscopy and Magnetism Laboratory does not end with the first functional prototype. Instead, the STM head can be redesigned and improved as new design and fabrication tools become accessible and new materials and design constraints are discovered. One such thing that became accessible to this project was metal 3D printing. When a metal 3D printer was available, the STM head design was updated to utilize the advantages of additive manufacturing and was fabricated. This chapter will focus on the future work that is being done and could be done using all the new tools that have become accessible since the start of the project. This new STM head design will also address and fix the issues faced with the subtractive manufactured STM head.

6.1 TRUMPF TruPrint 1000

TRUMPF TruPrint 1000 is a laser sintering additive production system capable of fabricating parts from various metals, such as titanium, stainless steel, aluminum, etc. The process by which this printer operates is called Selective Laser Melting (SLM), which involves a high-power laser to fuse small particles of metal into an object with predefined constraints.

SLM starts with a CAD model sliced into thin layers along a defined axis. This

layer height determines the quality of the printed part and can be adjusted in the slicing program. The thinner the slices are, the longer the print will take.

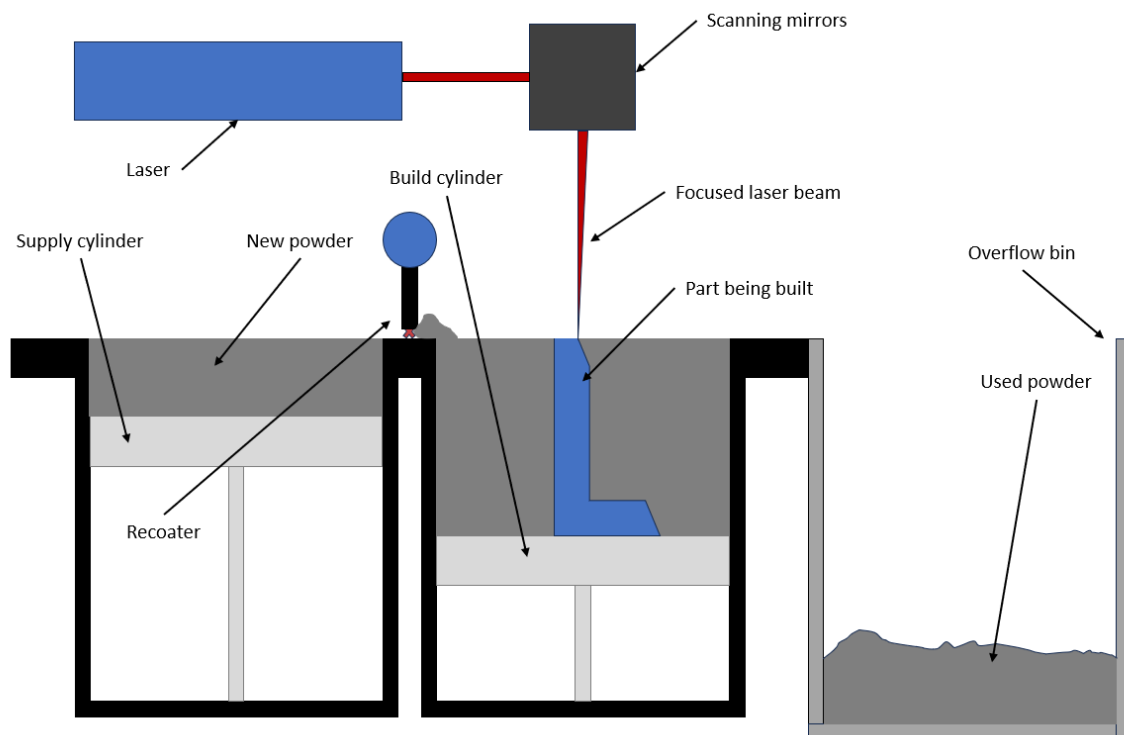


Figure 6.1: Cartoon of the layout inside the build chamber of TRUMPF TruPrint 1000. Here, the recoater moves a thin layer of powder from the supply cylinder to the build cylinder, and the laser melts this thin layer into the shape of the loaded part. All the extra powder the recoater carries is dumped into the overflow bin, and the process is repeated for the next layer.

The printing process can start once the sliced file is loaded into the printer. With the SLM method, a fine layer of power is initially applied to the build plate using a silicone recoater. Then, the laser selectively melts this powder in the shape of the initial slice made from the CAD file. The laser beam is directed by two high-frequency scanning mirrors, which help keep the focus on the build-plate while the beam moves around. The laser power is high enough to fully melt the metal powder to form the required solid structure. This process is repeated layer by layer to build the necessary part, and the layer height determines the amount of powder deposited by the recoater in each pass. This process occurs in an inert chamber with argon or nitrogen gas with oxygen levels below 100 parts per million.

TRUMPF TruPrint 1000 has a 200 W fibre laser and a beam diameter of $55\text{ }\mu\text{m}$ at the build plate. The build volume is a cylindrical shape of 100 mm in diameter and 100 mm in height.

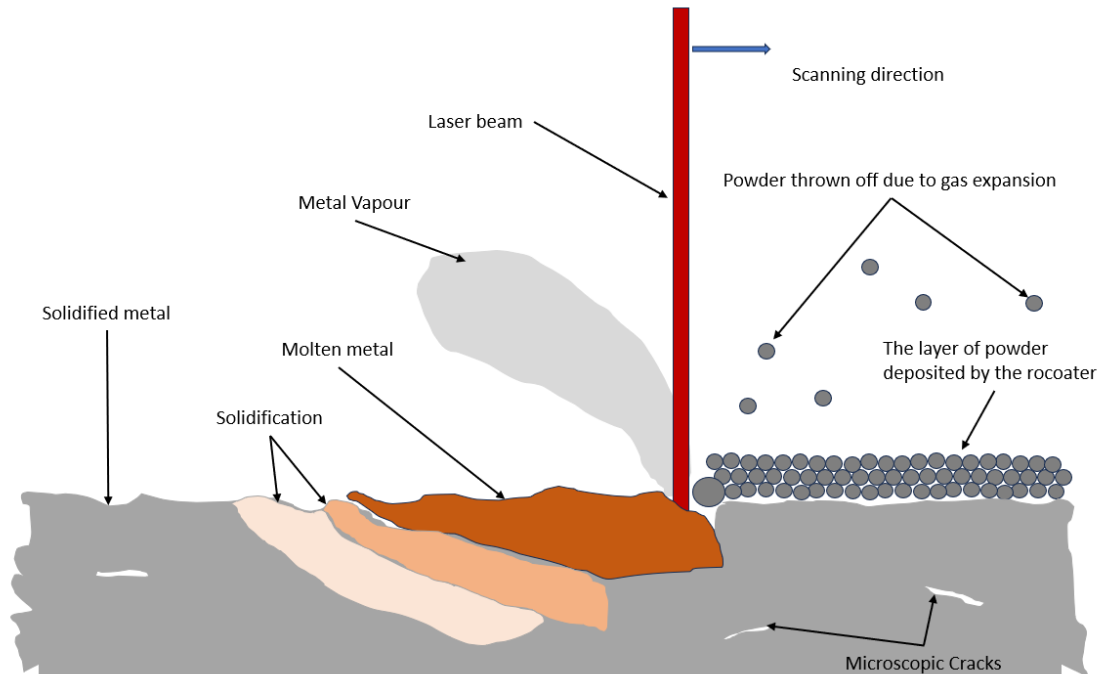


Figure 6.2: Detailed diagram of the procedure by which the metal powder is melted during the selective laser melting (SLM) process. The laser melting can lead to microscopic cracks and surface deformation that may affect the functionality of the final part if the print settings aren't ideal for the material [73].

6.2 Printable Materials

Some metals that can be printed using the TRUMPF TruPrint 1000 are stainless steel, aluminum, nickel-based alloys, tool steels, titanium alloys, and tungsten. One of the main conditions for printability is that the metal needs to exist in powder form. The metal powder used for printing must be in spherical form with low internal porosity for packing density and high flowability. The powder size is also very small, usually between $(20-63)\text{ }\mu\text{m}$, further improving flowability. Printing with titanium and tungsten powders broadens the capabilities of the STM by providing a stronger and more rigid material for the construction of the STM and a much higher heat-resistant metal for

sample preparation. SLM-printed titanium and tungsten have higher tensile strength than mill-annealed titanium, and annealing post-production can improve their ductility [74], [75]. Therefore, design structures could be made smaller without losing rigidity, and mass can also be reduced. Subtractive manufacturing processes, such as milling, can be difficult with harder materials like tungsten and rapidly wear out tools. In additive manufacturing, the process and wear and tear remain similar for most materials.

Furthermore, there have been a lot of studies on developing new superalloy powders for SLM printing [76], which could open more possible materials for the STM head that are better suited to the goals of this project.

6.3 Ti STM Head - Design Successor

The first prototype of the Ti STM is based on the Aluminum STM head made for this project. Therefore, it is a design made for subtractive manufacturing but later modified and improved for additive manufacturing. While designing the Ti STM, all the constraints for subtractive manufacturing, such as tool size, tool accessibility, and orientation of the features, do not apply. Therefore, the design parameters added to them could be dropped. This allowed the Ti STM head to have much smaller features for vibration dampening, and the choice of titanium over aluminum allowed the walls to be thinner while maintaining the rigidity and strength of the previous prototype.

Prism Cage One of the main changes made to the design was how the spring tension would be applied to the prism. Figure 6.3 shows that the beryllium copper leaf springs will be attached to a separate plate instead of the prism cage. This design allows the spring plate to be adjustable, thus adjusting the spring force on the prism. This would also allow for the easier installation of the prism in the prism cage, as one of the cage inserts can be installed through the cutout at the spring plate after the prism is installed.

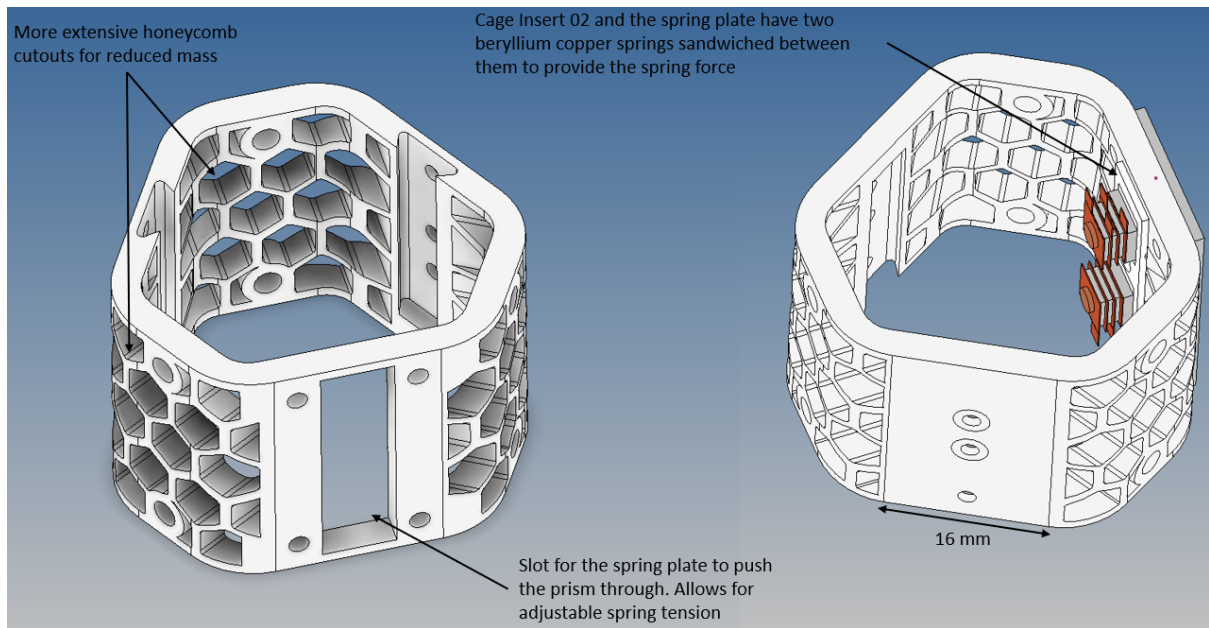


Figure 6.3: Titanium prism cage that has thinner walls and a more extensive honeycomb pattern to reduce mass while preserving rigidity. It also has a slot for the springs from the spring plate to provide tension for cage insert 02 and the prism. Spring plate assembly is also shown here.

Prism: The prism in this design also has honeycomb pattern cutouts to reduce mass while preserving rigidity. This was impossible in the aluminum design as the cutout made the aluminum part too fragile to handle without deforming during the assembly process.

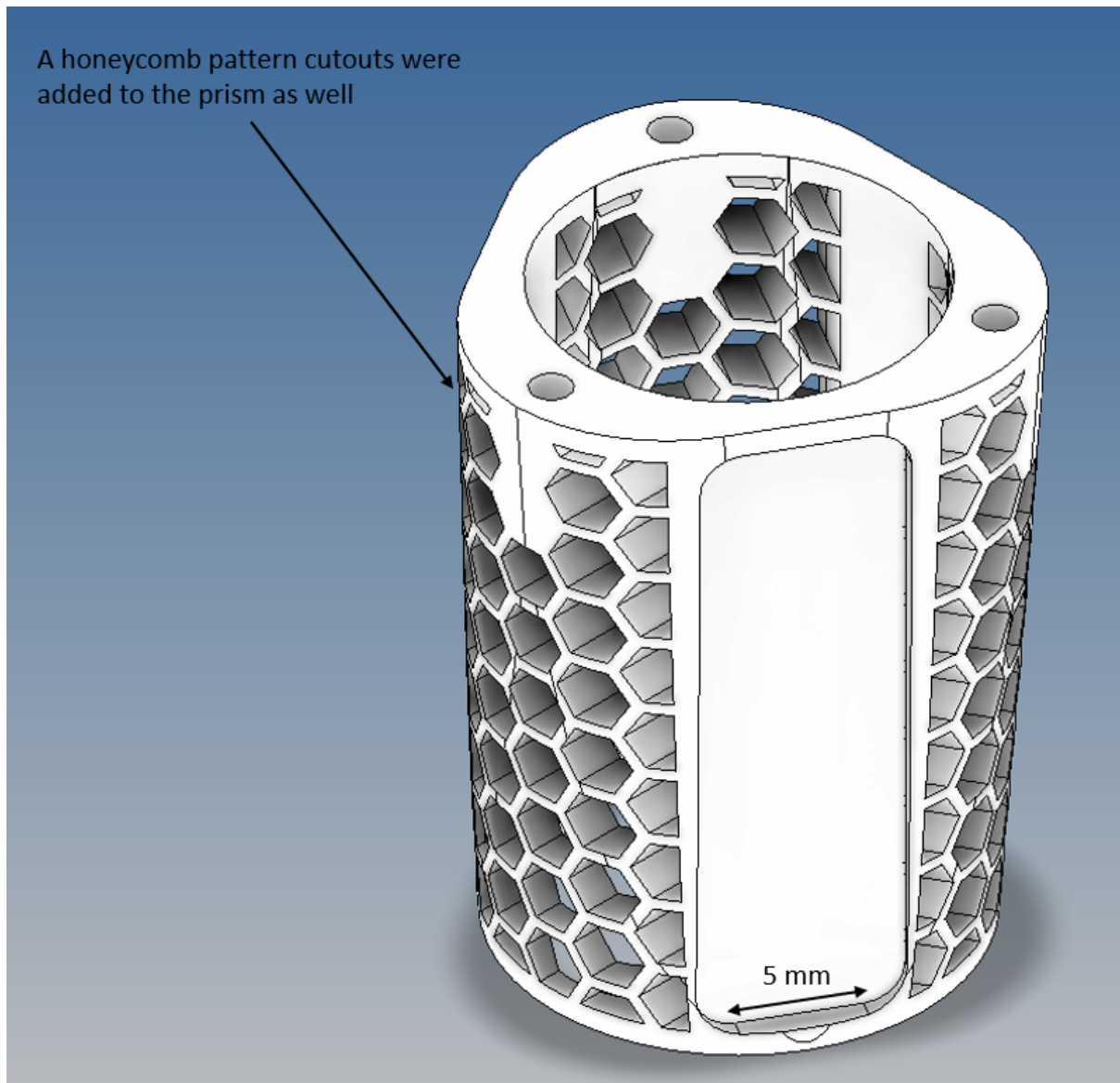


Figure 6.4: The titanium prism with a honeycomb pattern cutout to reduce mass, similar to the prism cage. The walls are also made thinner since titanium is stronger than aluminum.

Prism Cage Inserts: The prism cage inserts can have the dovetail design extending to the height of the inserts, as tool length limitations are no longer a problem. This also allows the cage inserts to be much more stable and rigid once installed. The assembly procedure for the cage inserts has also improved as they can be aligned and kept in the dovetail cuts of the prism cage easily due to the tighter tolerances of 3D printing and the full-length dovetail design.

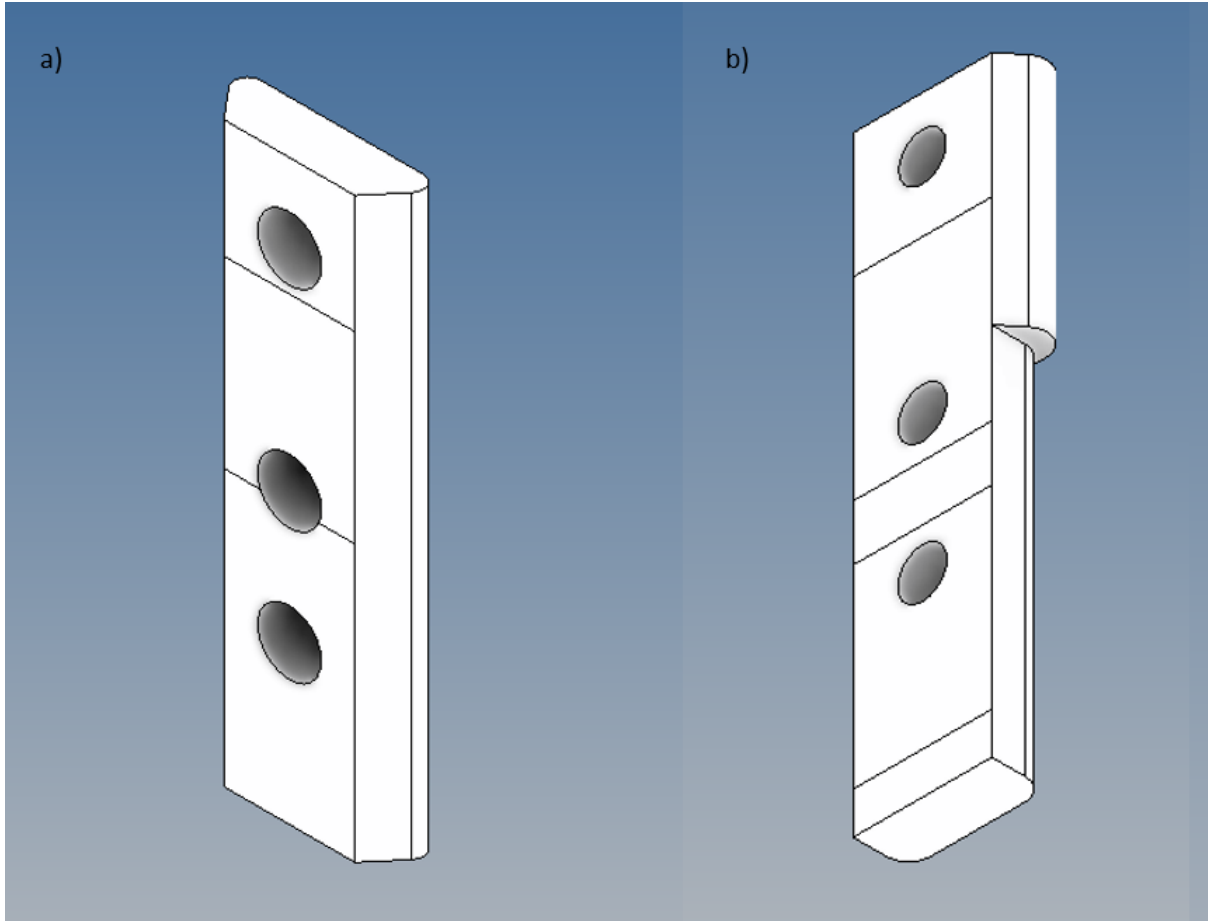


Figure 6.5: Titanium prism insert [a)] compared to the Aluminum insert [b)]. The aluminum insert has the dovetail design going only partway down its length due to machining constraints, whereas the titanium insert's dovetail goes all the way down.

STM Head Legs: Incorporating additive manufacturing also opens many design options that were not available before. One of the main features we are interested in is generative design. Unlike conventional CAD workspaces, in generative design, we set the goals and constraints of the design first and let AI algorithms come up with various designs from which we can pick. The Ti STM head legs were designed using this process, and as we can see in Figure 6.6, the design is too complicated for subtractive manufacturing. Therefore, this process is only ideal for additive manufacturing.

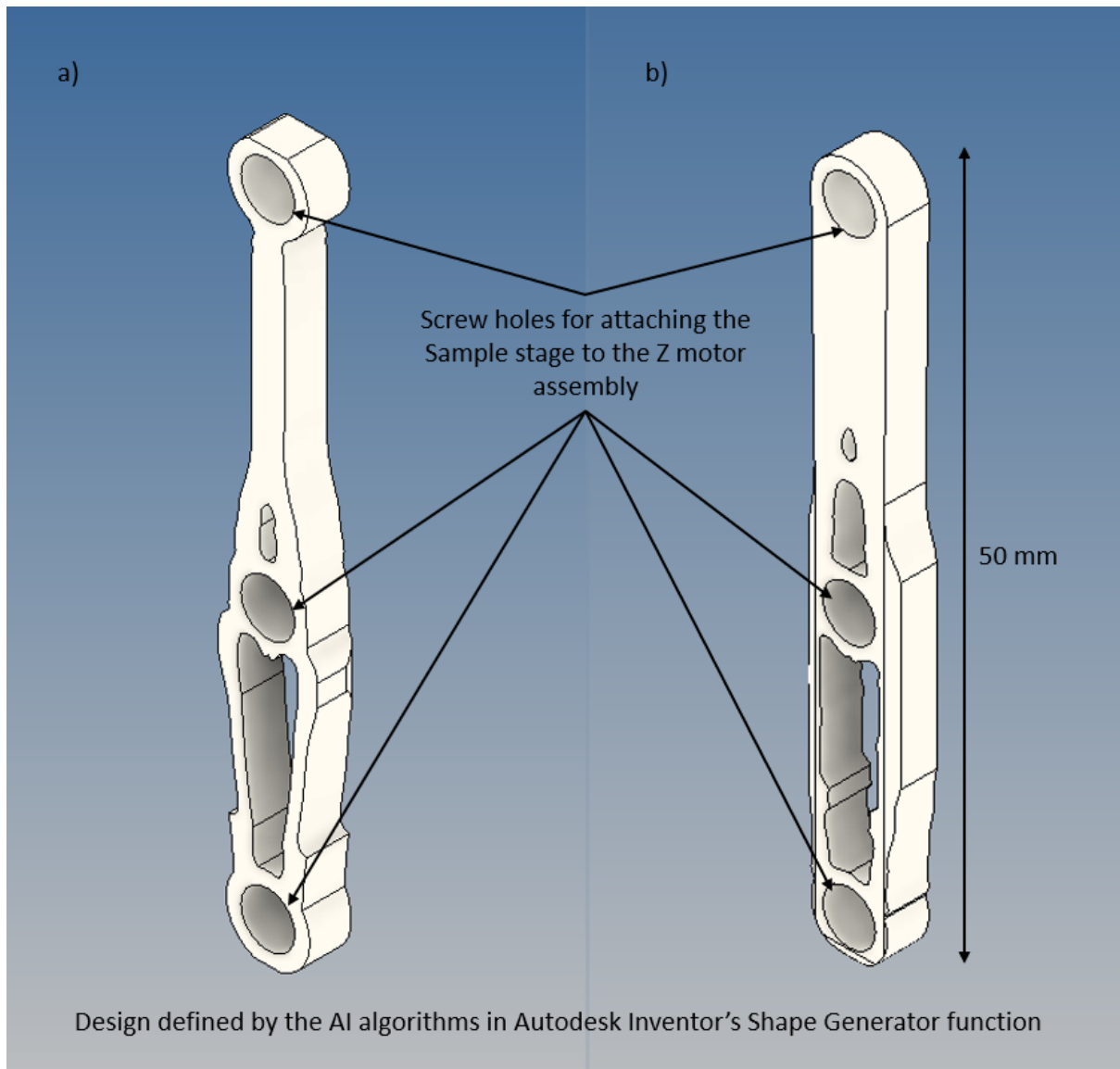


Figure 6.6: Titanium STM head legs designed using the AI algorithms available via the shape generator function in Auto-desk Inventor Professional 2023. The constraints were set to maximize the normal modes while the design was grounded at the screw holes.

Sample Cage: The sample cage had the most changes made to its design in this version of the STM head. This was because it was one of the primary sources of the lowest normal modes, and as it was the largest part of the assembly, it could lose the most mass through design alterations. The honeycomb pattern cutouts were incorporated into the sample cage design to help reduce mass wherever a solid wall wasn't needed, as shown in Figure 6.7. The corners of the sample holder were made more robust to improve the rigidity of the structure.

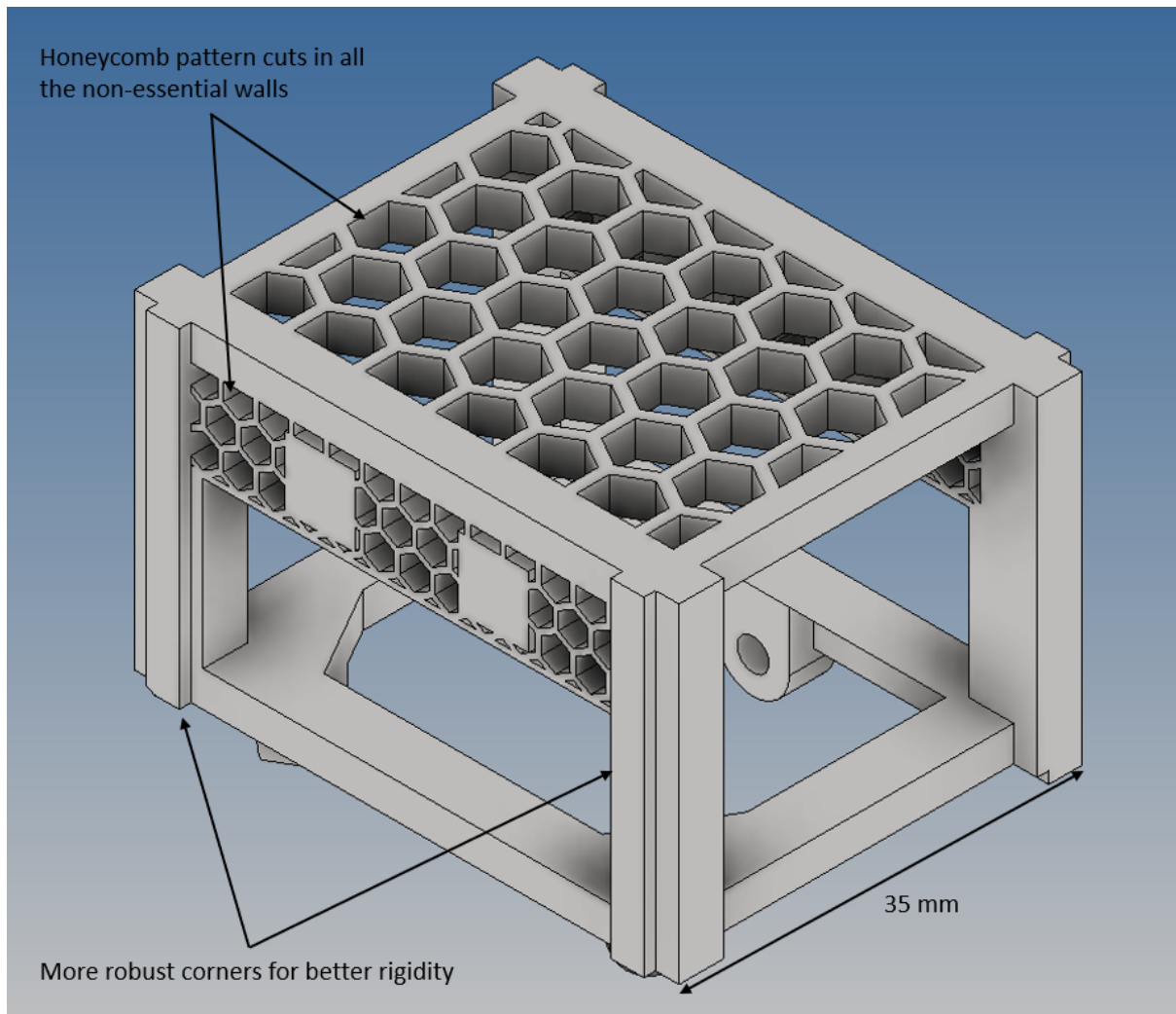


Figure 6.7: Titanium sample cage modified to have a lower mass while preserving rigidity and strength. Corners are made more robust to increase the normal modes and improve rigidity.

Other components of the STM head: Minor changes were made to the rest of the STM head parts, or the same design was kept for this prototype.

Future Design: For the Ti STM head to utilize all the advantages offered by additive manufacturing, the head must be redesigned from the ground up instead of modifying the current STM head. This will allow us to incorporate generative design features more into the design process and help us move away from the conventional design styles. More complex design features that were avoided due to the difficulty in the machining process can now be implemented and tested in the design. FDM printing of prototypes will also be a better test of the design since the manufacturing

process for the final parts will be similar.

6.3.1 Resonant Modes

Resonant mode analysis was also done for the Ti STM head design, which is similar to the subtractive-manufactured STM. Figure 6.8 compares the resonant modes of both STM head designs. The lowest mode for the Ti STM head (1172 Hz) is higher than the lowest mode (1116 Hz) for the aluminum head. However, we can see that the aluminum STM has higher resonant frequency amplitudes between modes 2-10. The Ti STM head is still preferred as the lowest resonant mode will impact the STM head stability the most. The generative design will help increase the lowest resonant modes even further for the next additive-manufactured head prototype.

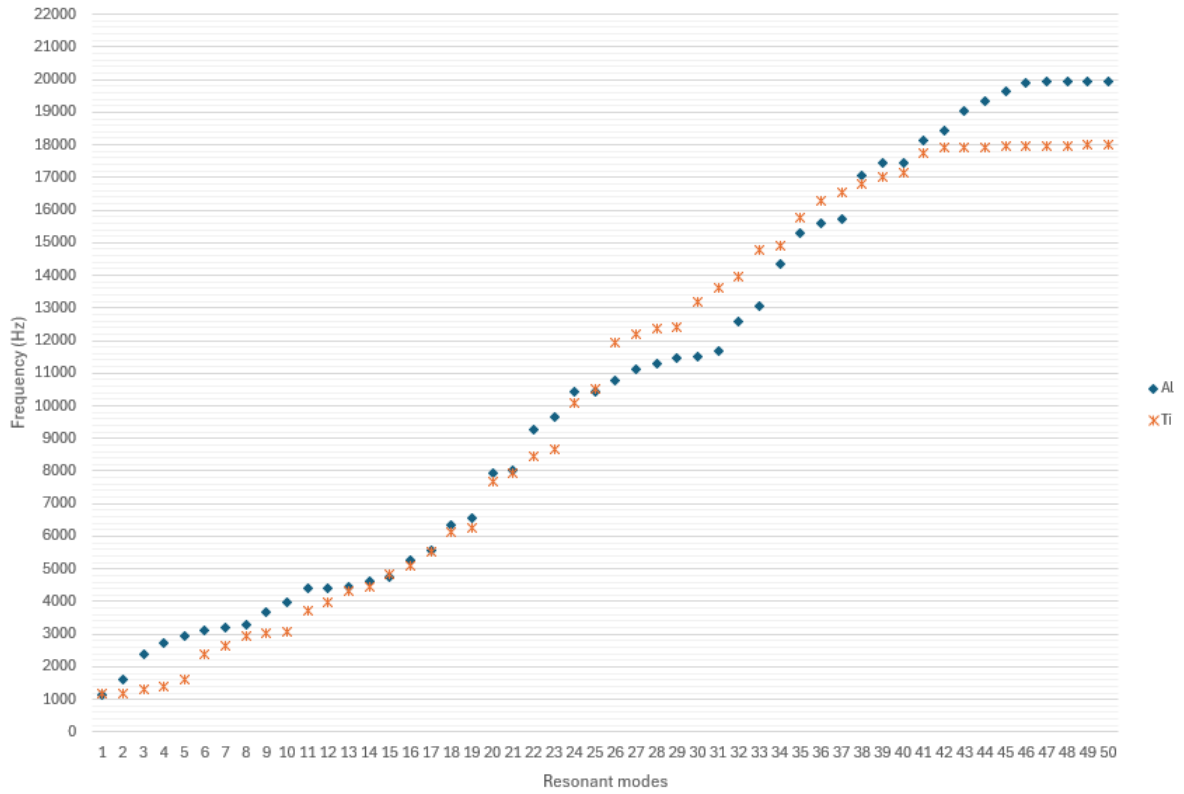


Figure 6.8: The first fifty resonant modes of the additive-manufactured (Ti) and the subtractive-manufactured (Al) STM head compared.

DIRECTION	TOTAL (kgm ²)	MODAL (kgm ²)	PERCENT
1	7.03e-04	6.13e-04	87.2298
2	7.03e-04	6.23e-04	88.7376
3	7.03e-04	6.31e-04	89.8674
4	1.45e-03	1.38e-03	95.4792
5	2.99e-04	2.48e-04	83.2862
6	1.49e-03	1.41e-03	94.6482

Table 6.1: The percent modal mass of the additive-manufactured STM head design was kept above 85% to improve the accuracy of the calculated resonant modes.

6.4 UHV Compatibility and Testing

There are two major 3D-printing processes used for printing metal: binder jet 3D printing and selective laser melting (SLM). In binder jet 3D printing, an inkjet printer deposits a thin layer of binding agent, and then a layer of metal powder is added onto it, and this process is repeated in layers until the part is created. Once the part is finished, the unbound powder is melted and removed in a furnace. This process is not ideal for vacuum compatibility as it leaves the parts porous and with low density, leading to outgassing in vacuum environments. Meanwhile, in SLM printers, the metal powder is directly melted into the desired shape by a high-powered laser, layer by layer, to build a part. This allows the part to have a dense and solid structure with very little to no pockets for trapped air within the part body and is ideal for vacuum compatibility.

3D-printed titanium made from SLM printers is already shown to be UHV compatible in other tests [77] if the print process is conducted correctly. However, incorrect printing parameters can leave cracks and pockets under the surface that could be a source for outgassing once placed in a UHV environment. Therefore, to test our printing parameters, two 3D-printed titanium rings were placed in the vacuum chamber at high vacuum to see if there were any changes to the chamber pressure from the ring's presence. No changes to the chamber pressure were seen, leading us to conclude that the titanium printing parameters were correct. The next step is to check for UHV compatibility with the printed tungsten parts.

Chapter 7

Conclusion

7.1 Conclusion

The primary design objectives of this STM, which are being non-magnetic, having high rigidity, UHV compatibility, high resonance modes, and optical access to the tunnelling junction, are successfully met. The current design for the STM head fits in an extremely small footprint and is able to fit in its allocated slot in the scan chamber as well. High resonance modes were achieved using NASTRAN analysis to calculate the resonance modes and adjust the design to increase the modes to the desired levels. The piezoelectric stacks made for the STM were also tested and shown to work. However, when connected to the STM head controller, the z-motor could not provide coarse walking due to the inability to adjust the beryllium copper leaf spring tension and the piezoelectric stack wires shorting. Since the problems with the z-motor are isolated, they will be fixed in the next version of the STM head. Furthermore, the UHV chambers have all been assembled and tested.

The next steps to finishing the STM head are to test the cold head for the STM and assemble the additive-manufactured Ti STM head.

In conclusion, most of the project's targets have been successfully met. Although the STM's z-motor does not function, the issue has been identified and is being addressed.

7.2 Design Choices and Future Improvements

One of the major outcomes of this project, which will help with the rapid prototyping and improvements of future STM heads for the Ultrafast Microscopy and Magnetism laboratory, is the workflow created to produce the STM heads. This workflow starts with a prototype, initially 3D printed out of plastic to test for compatibility, and then it is transferred to Autodesk NASTRAN for normal mode analysis. Here, the design is altered depending on which parts of the STM head are responsible for the lowest normal modes and re-analyzed with NASTRAN. After multiple design and analysis cycles, the design is sent for fabrication once the lowest normal mode is at an acceptable value.

Initially, fabrication was done using a 5-axis CNC mill, but now we are stepping into a new era with fabrication being done using a metal 3D printer. Once the parts are fabricated, they will be assembled and tested for their normal modes and coarse walking. This workflow not only enhances the design of the STM but also opens new avenues for adding additional features to the STM. Moreover, it enables the efficient production of custom STM heads for studying specific samples, sparking new possibilities in our research.

Subtractive manufacturing and the Pocket NC mill were the primary constraints that dictated the design choices for the current STM head. However, the components were all still compact and lightweight and had high enough resonant frequencies to conform to the design goals initially set out for this project. The two major problems with this design that prevented it from coarse walking have also been identified and resolved in the Ti STM head that supersedes the current design.

The sample holder design still needs to be revised and improved. Using additive manufacturing will help speed up the design and prototyping of the future sample holder design. Once the next STM head prototype is ready, it must be tested for coarse walking and UHV compatibility. All the next prototype's components are fabricated and waiting to be assembled for testing.

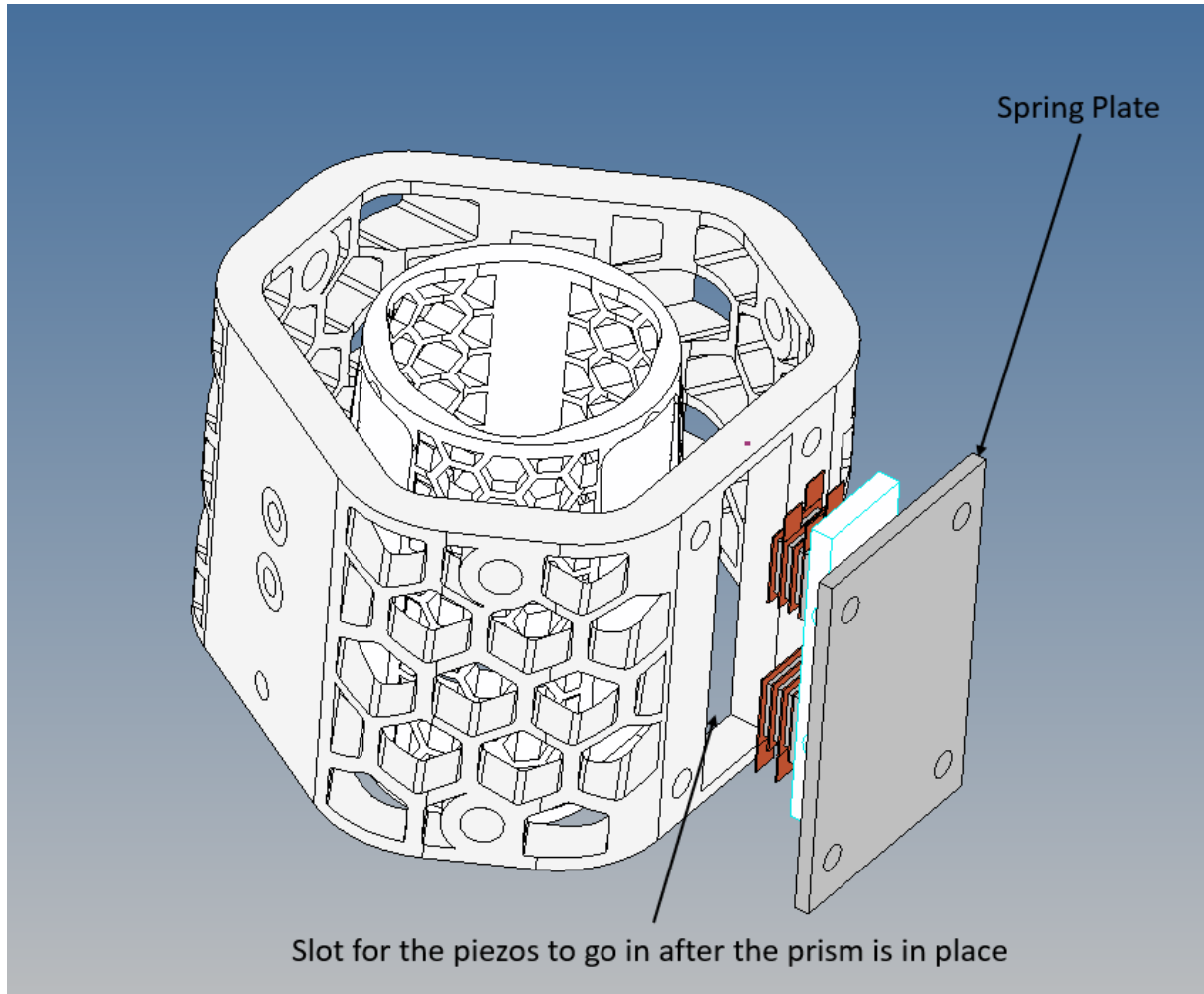


Figure 7.1: The process of inserting the third prism cage insert to provide the necessary spring force required for the stick-slip motion. The spring plate will be attached to the prism cage with screws that allow for the adjustment of the spring tension. There will be springs around the screws to provide the spring force.

7.2.1 Generative Design

The second Ti STM head prototype will be fully designed using generative design functions available through Fusion 360. This will allow us to take advantage of all the benefits of additive manufacturing. Generative design harnesses artificial intelligence (AI) to develop new, highly latticed designs with intricate features based on predefined constraints. One significant advantage of generative design is that it explores and compares thousands of design iterations in a very short period of time to come up with the best results for the given goals. This would allow us to skip several prototypes that otherwise would have made it to the final design stages for the new STM head and save significant design time.

Generative design algorithms often create highly efficient organic shapes ideal for 3D printing. The lattice structures made by generative design are also something a human engineer would not come up with, and they take full advantage of the design freedoms offered only by 3D printing technologies. Therefore, incorporating generative design into the STM head workflow would significantly speed up the new STM head turnover time and help advance the head design.

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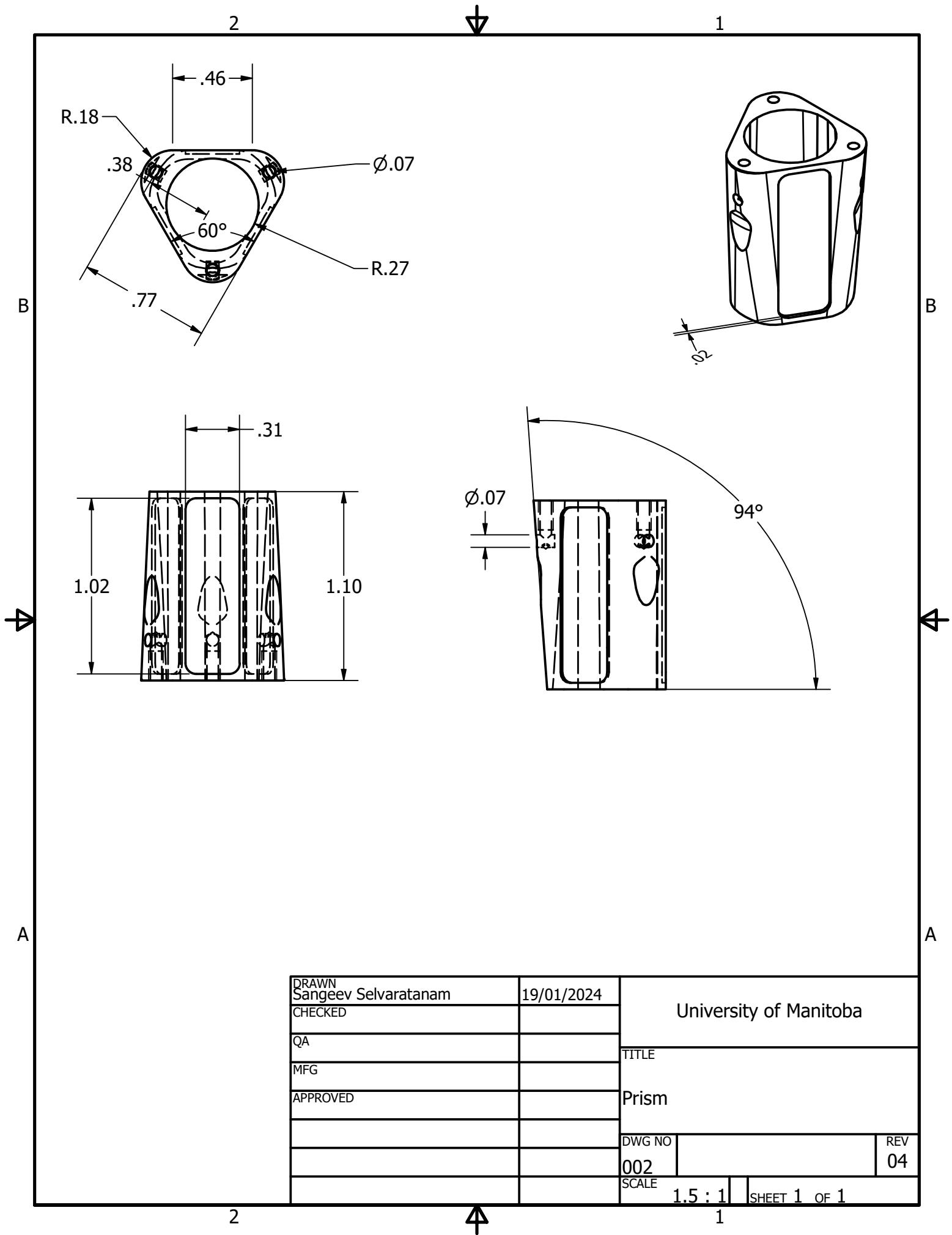
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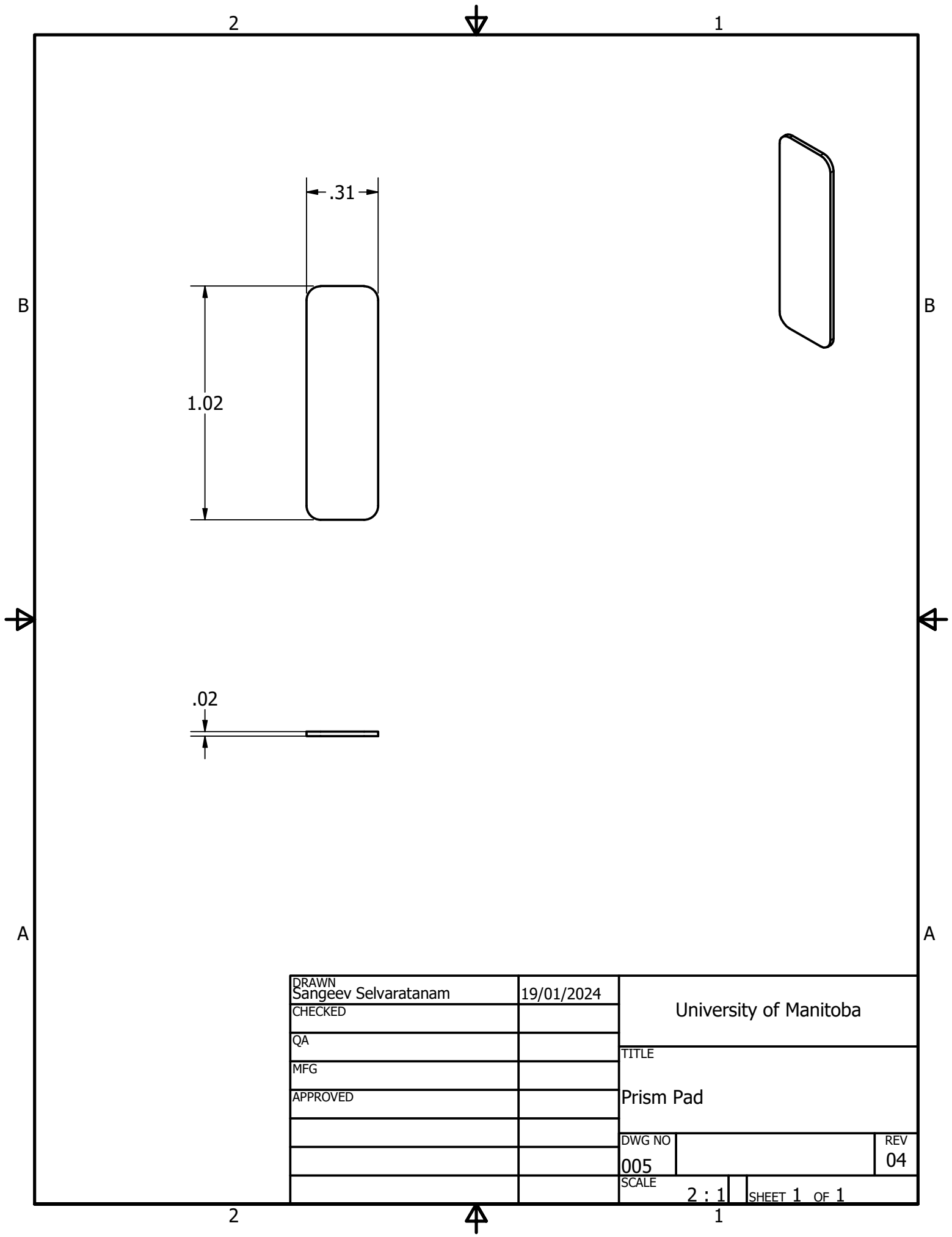
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Appendix A

Part Drawings

Detailed drawings of all the components in the STM head are presented in this Appendix. 3D versions of these files are available upon request. The drawings contain all the required dimensions of each for the parts to be recreated. All dimensions are given in millimetres unless otherwise specified.



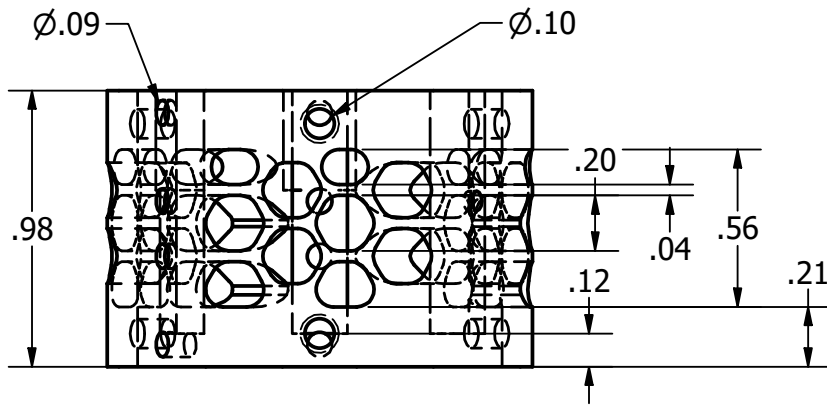
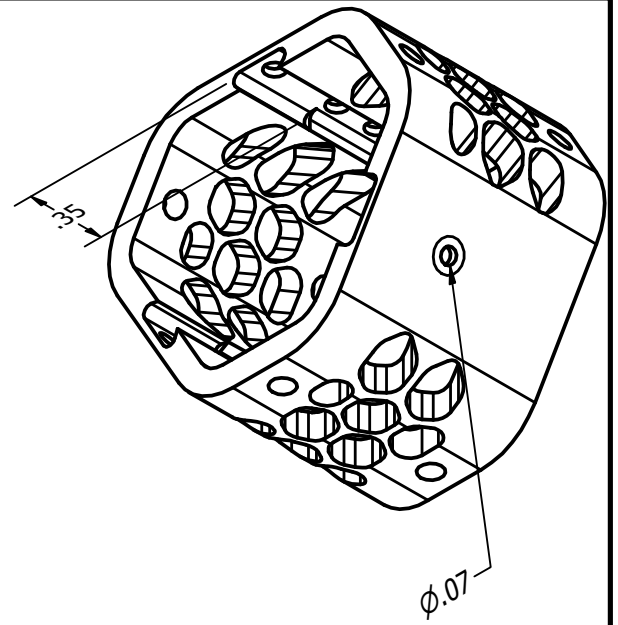
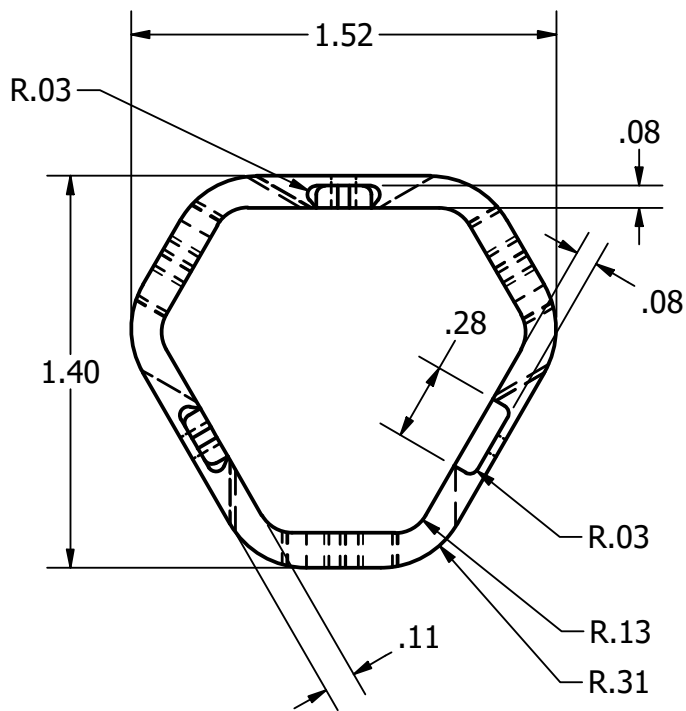


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MFG					
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2



1



B

B

A

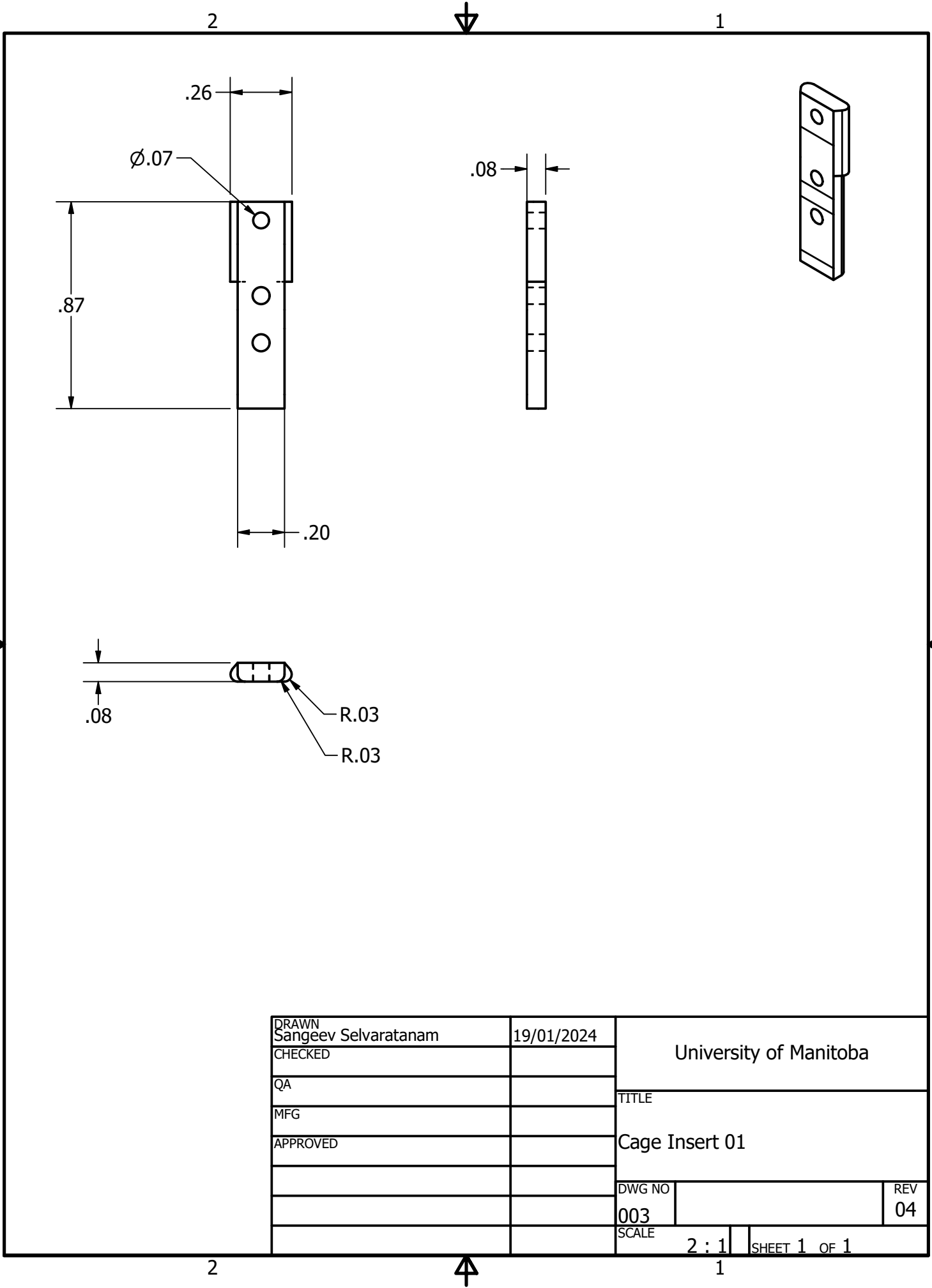
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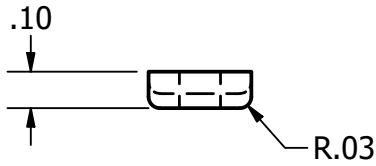
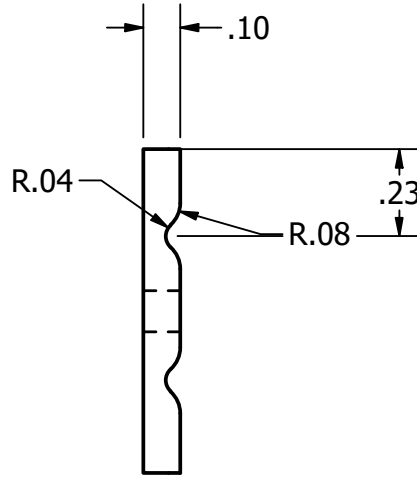
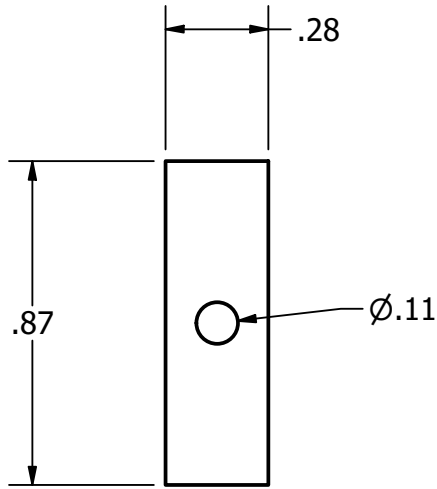
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2

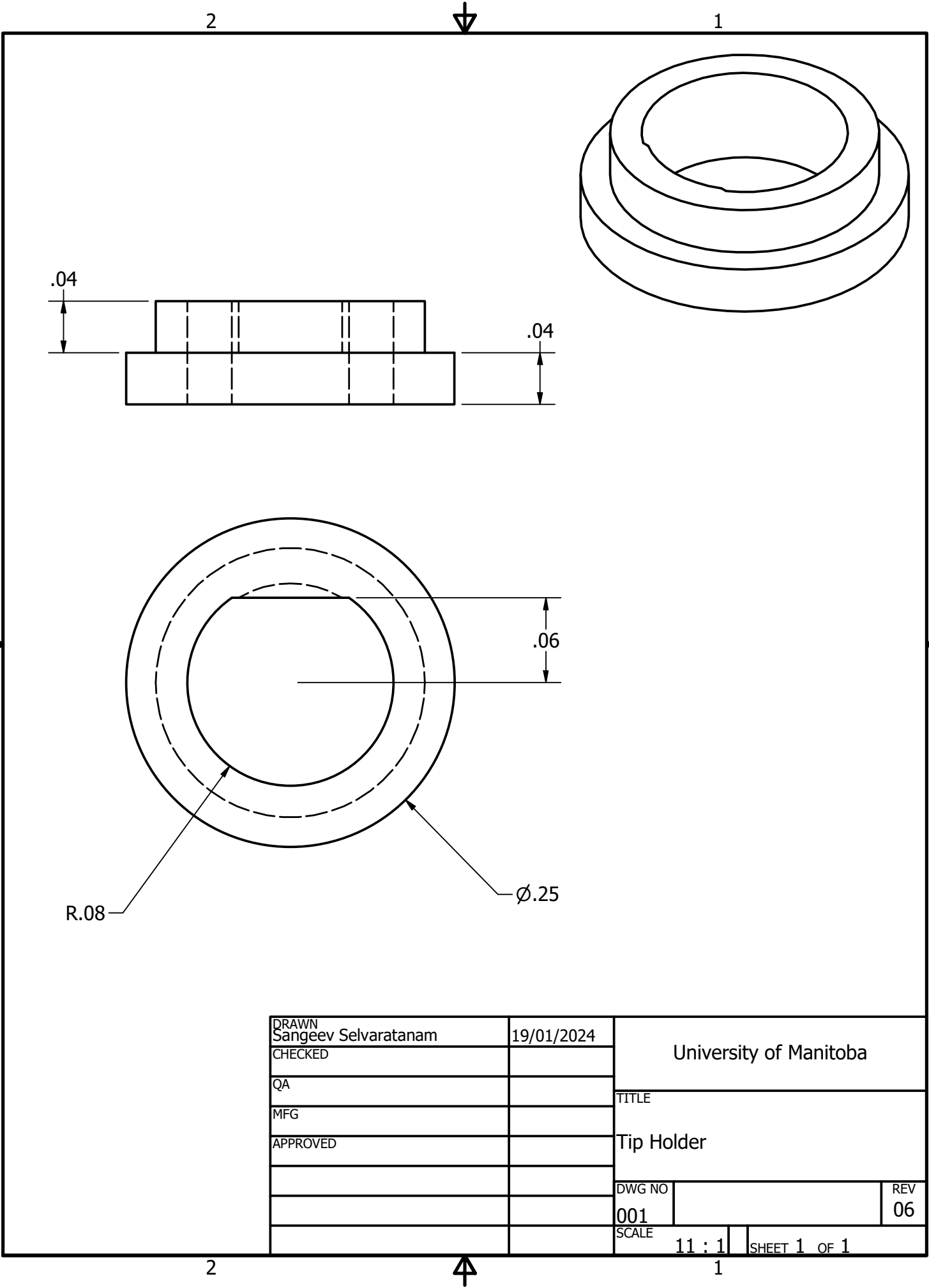


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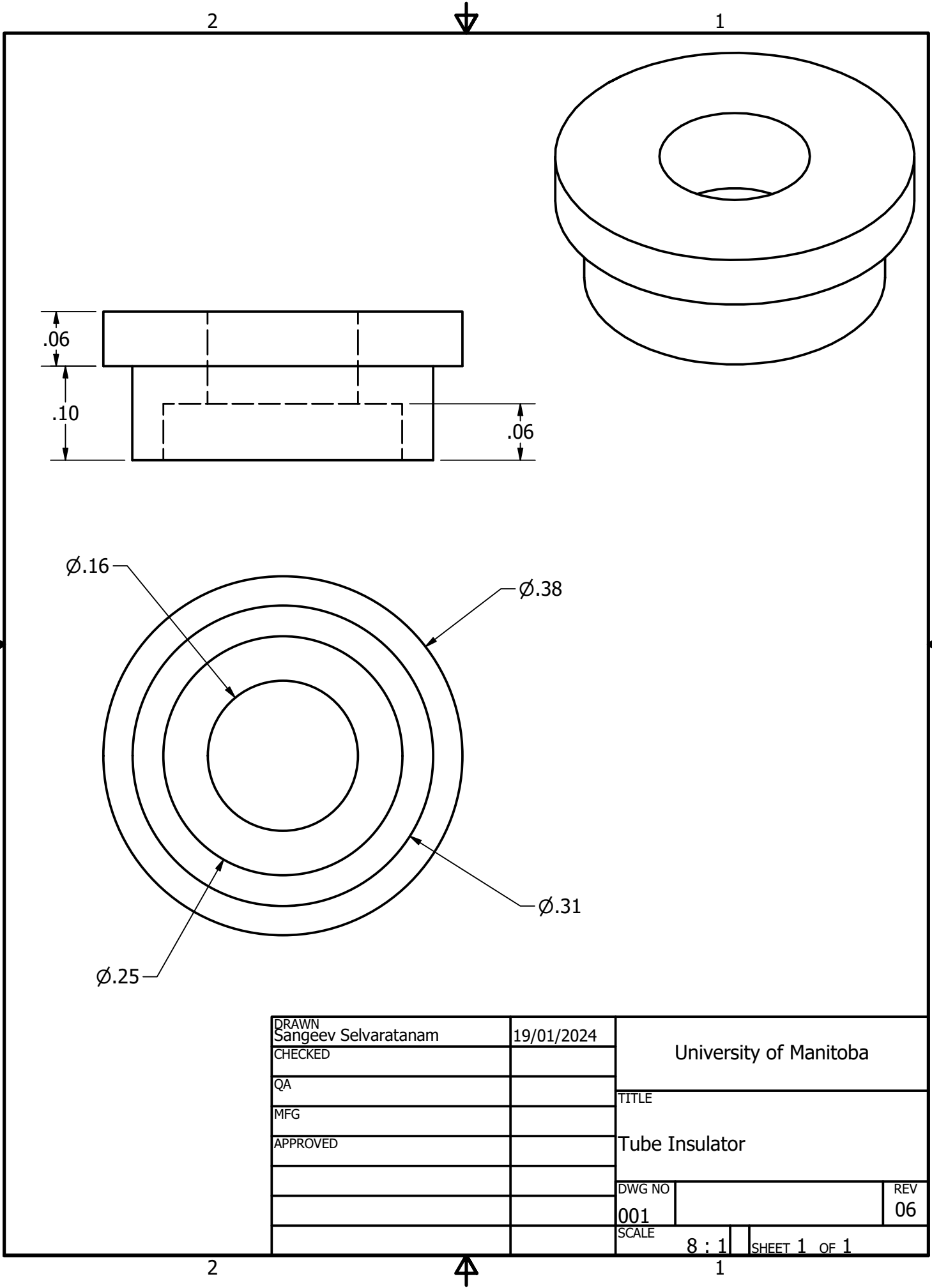




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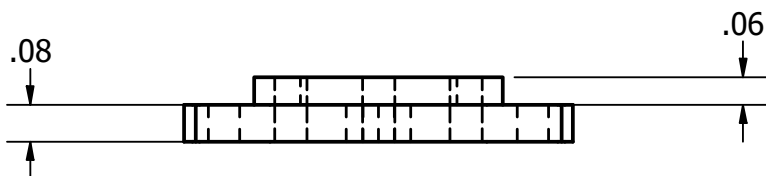
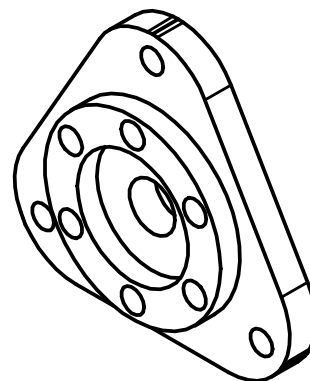
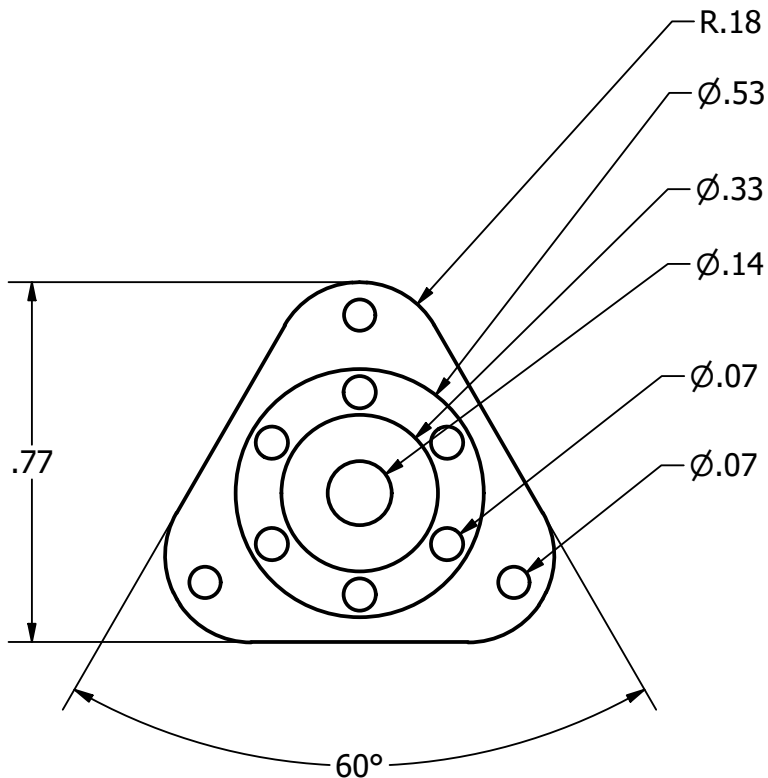


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B

B



A

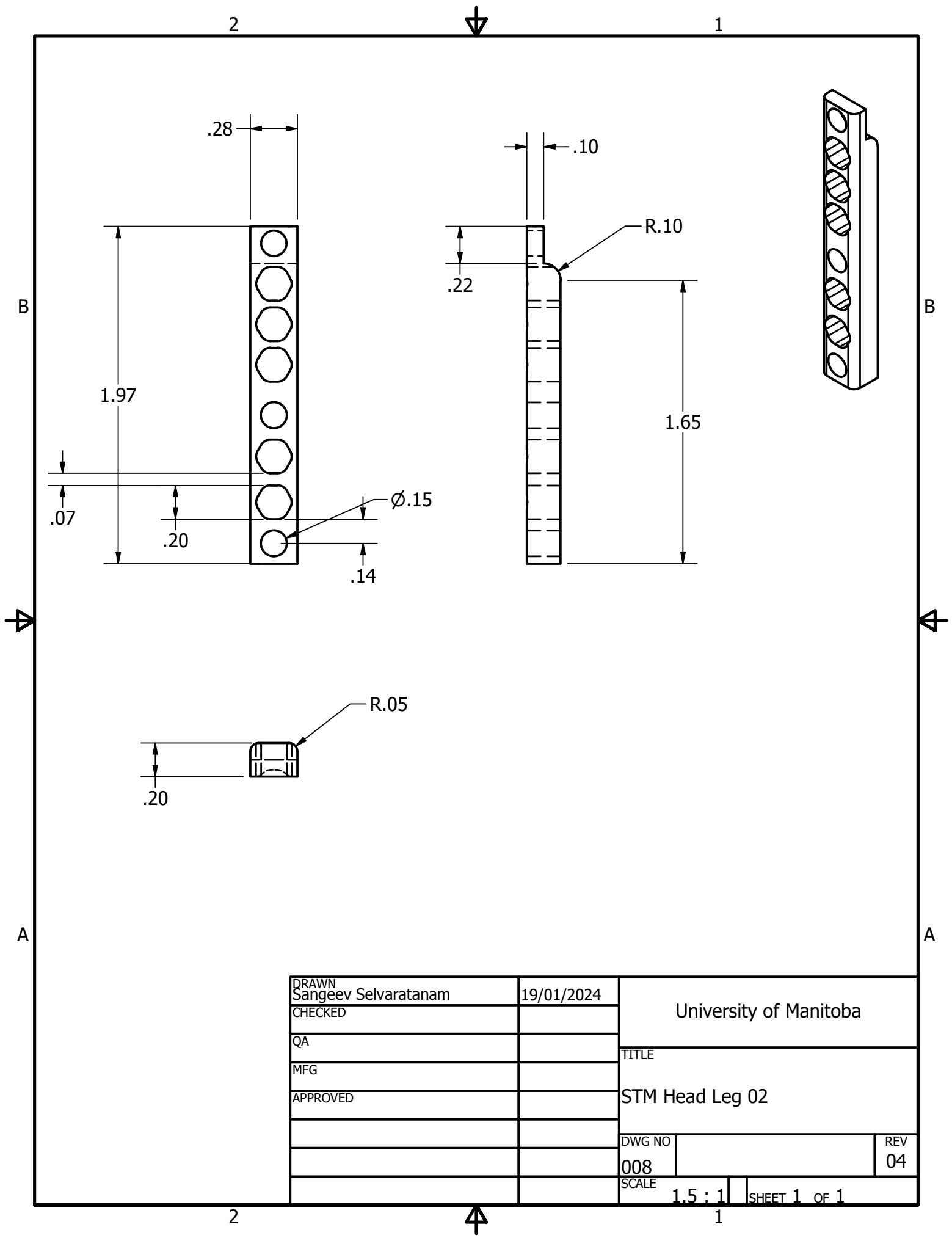
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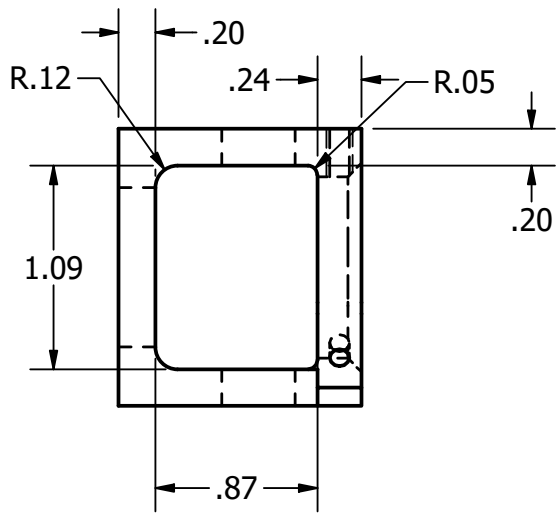
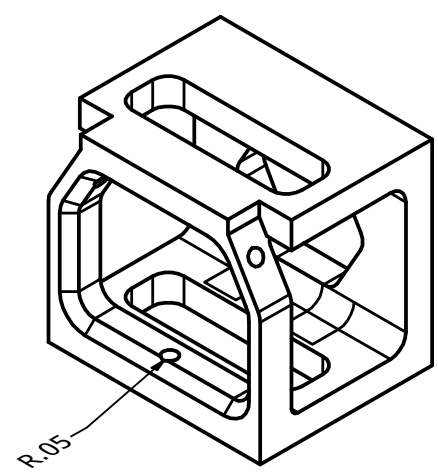
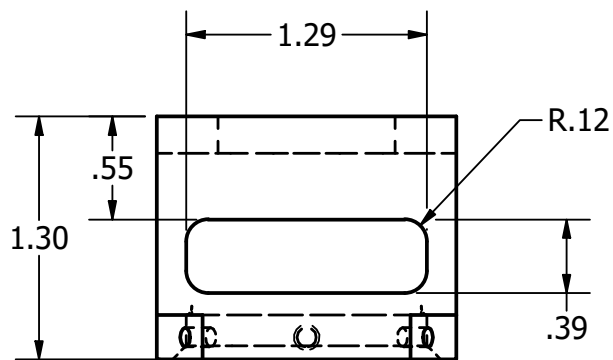
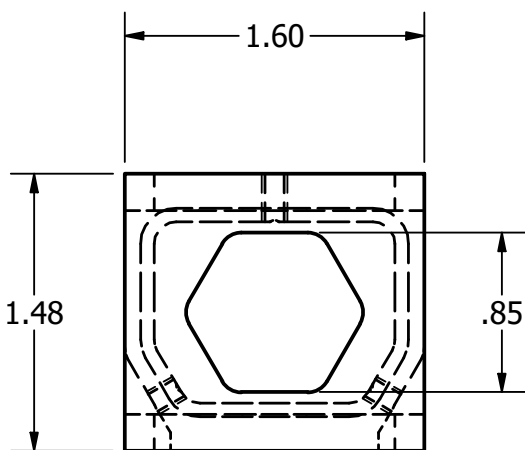
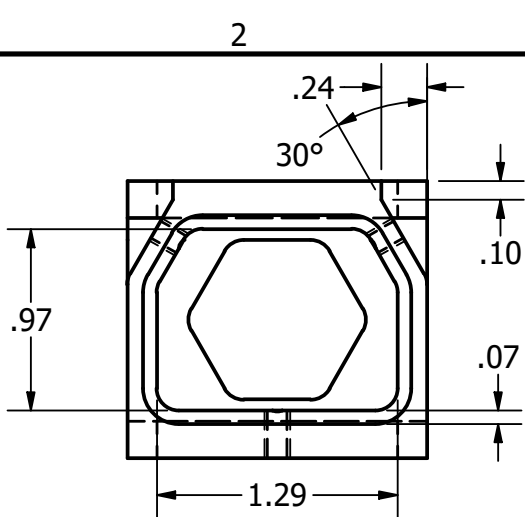
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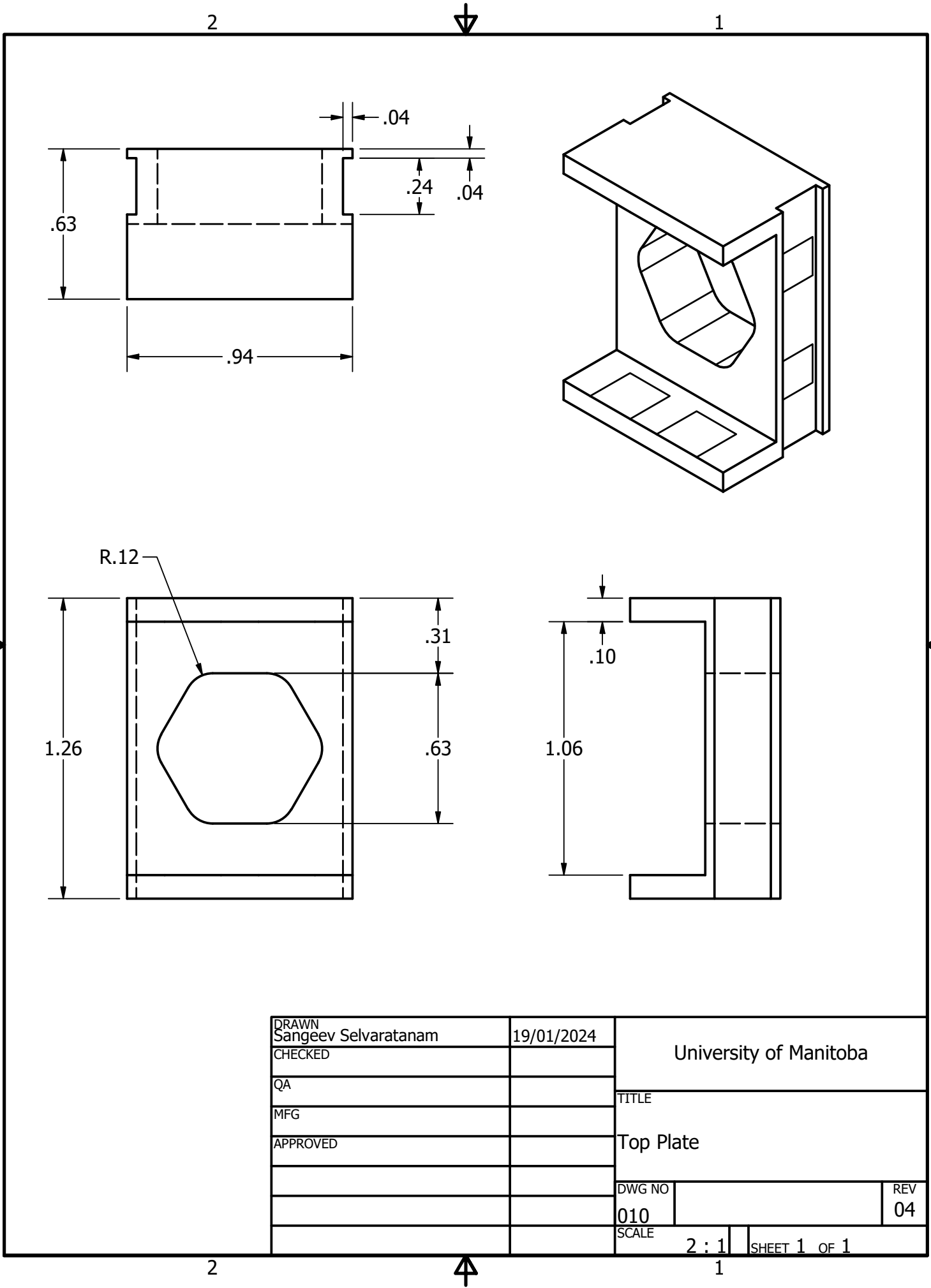


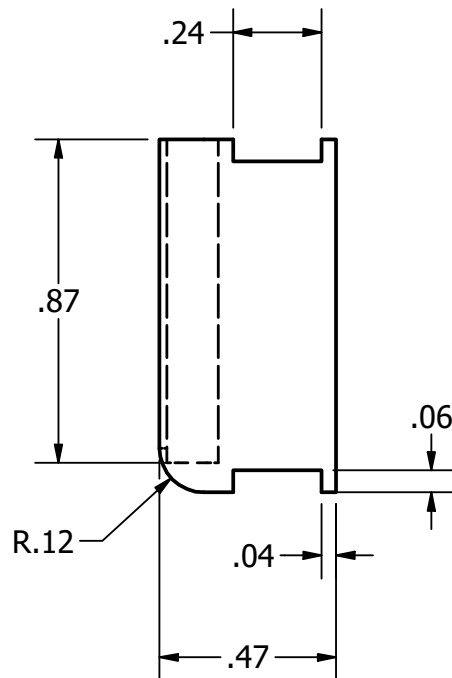
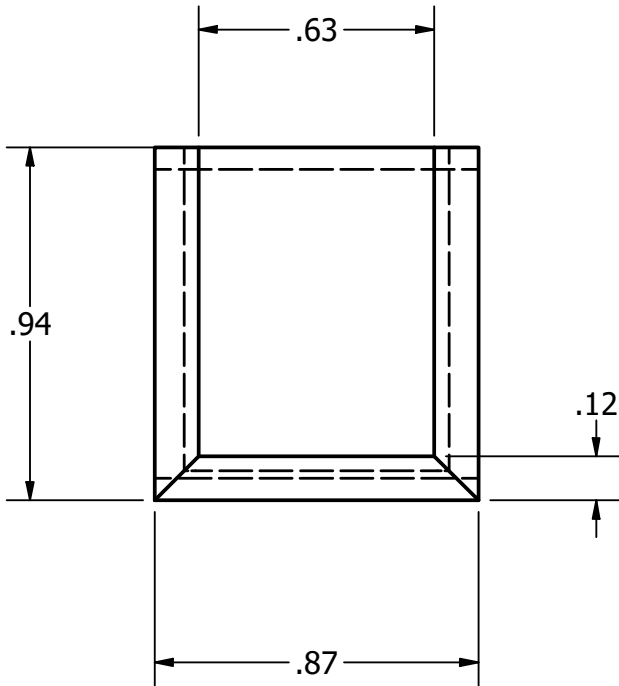
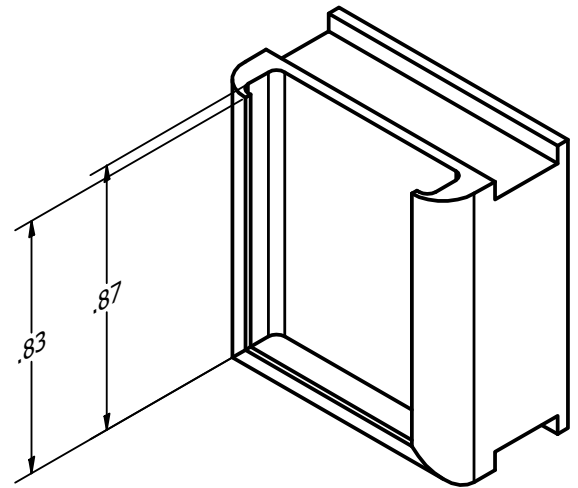
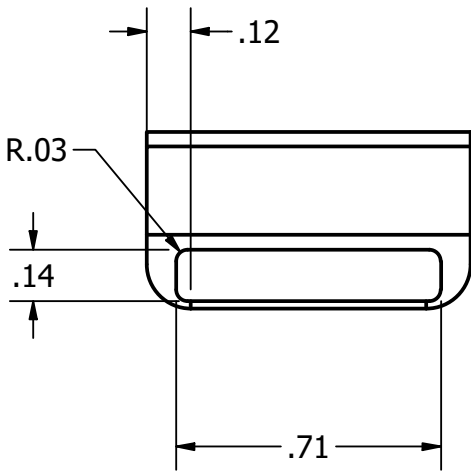


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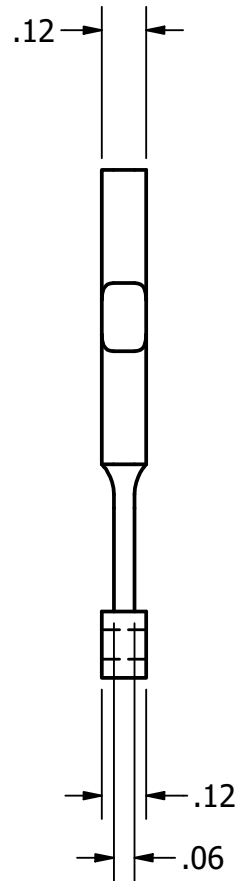
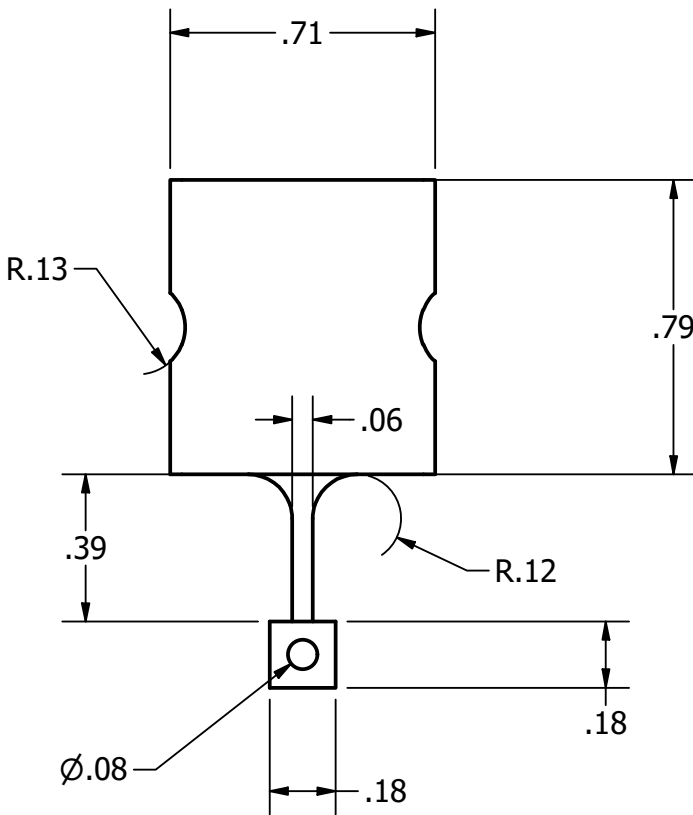
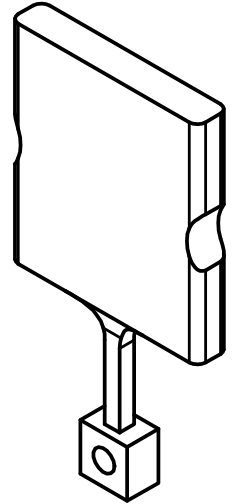
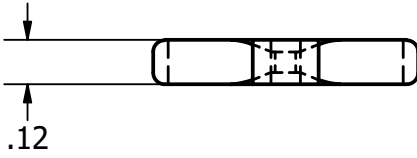




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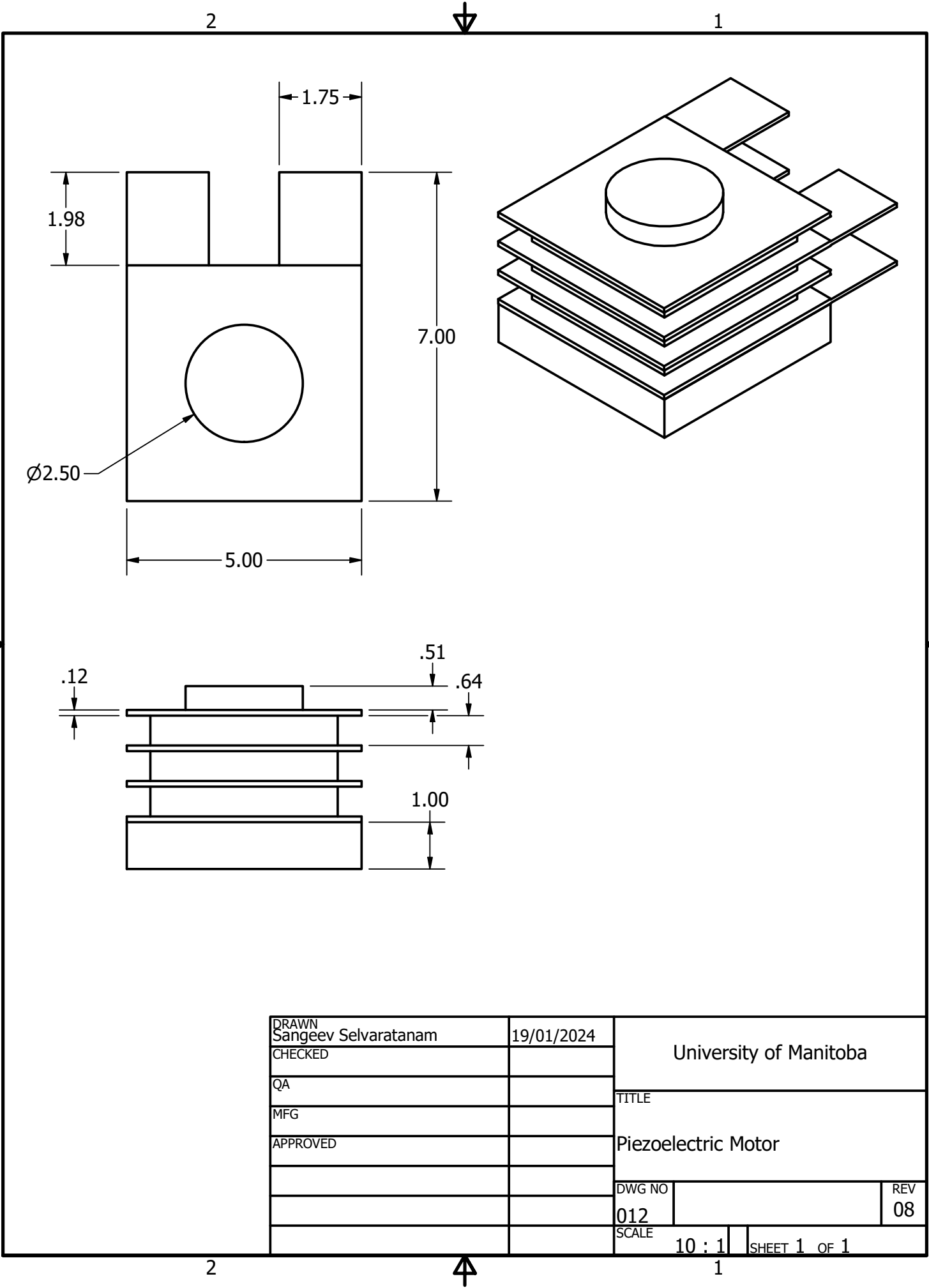
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2

1



DRAWN	Sangeev Selvaratanam	19/01/2024	University of Manitoba		
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MFG					
APPROVED			Piezoelectric Motor		
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Appendix B

PocketNC Settings

The following settings are ideal for the carbide end mills used on aluminium in the Pocket NC V2-10 5 axis CNC mill. These settings were tried and tested with Autodesk Fusion 360, and it is recommended to apply some cutting fluid for the rough passes every 15-20 minutes. The aluminium tends to gum up on the tool, and this could lead to tool breakage if sufficient cutting fluid is not used. Cutting fluid is not necessary for the final passes.

Spindle Speed	8500 rpm
Ramp Spindle Speed	8500 rpm
Cutting Feedrate	13 in/min
Lead-in Feedrate	3 in/min
Lead-out Feedrate	5 in/min
Ramp Feedrate	3 in/min
Plunge Feedrate	5 in/min
Optimal Load	0.0125 in
Maximum Roughing Stepdown	0.15 in
Radial Stock to Leave	0.02 in
Axial Stock to Leave	0.02 in

Table B.1: Rough pass speeds and feedrates for a 1/4" 4 flute roughing end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	13 in/min
Lead-in Feedrate	3 in/min
Lead-out Feedrate	5 in/min
Ramp Feedrate	3 in/min
Plunge Feedrate	5 in/min
Optimal Load	0.0125 in
Maximum Roughing Stepdown	0.15 in
Radial Stock to Leave	0.02 in
Axial Stock to Leave	0.02 in

Table B.2: Rough pass speeds and feedrates for a 1/8" 2 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	13 in/min
Lead-in Feedrate	3 in/min
Lead-out Feedrate	5 in/min
Ramp Feedrate	3 in/min
Plunge Feedrate	5 in/min
Optimal Load	0.008 in
Maximum Roughing Stepdown	0.15 in
Radial Stock to Leave	0.02 in
Axial Stock to Leave	0.02 in

Table B.3: Rough pass speeds and feedrates for a 1/8" 4 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	5 in/min
Lead-in Feedrate	3 in/min
Lead-out Feedrate	5 in/min
Ramp Feedrate	4 in/min
Plunge Feedrate	5 in/min
Maximum Stepdown	0.0078 in
Radial Stock to Leave	0 in
Axial Stock to Leave	0 in

Table B.4: Final pass (Ramp toolpath) speeds and feedrates for a 1/8" 4 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	5 in/min
Lead-in Feedrate	3 in/min
Lead-out Feedrate	5 in/min
Ramp Feedrate	4 in/min
Plunge Feedrate	5 in/min
Radial Stock to Leave	0.02 in
Axial Stock to Leave	0 in

Table B.5: Final pass (Parallel toolpath) speeds and feedrates for a 1/8" 4 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	8500 rpm
Cutting Feedrate	0.1 in/min
Lead-in Feedrate	0.1 in/min
Lead-out Feedrate	0.1 in/min
Ramp Feedrate	0.1 in/min
Plunge Feedrate	0.1 in/min

Table B.6: Boring holes speeds and feedrates for a 0.062" 3 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	8500 rpm
Cutting Feedrate	0.15 in/min
Lead-in Feedrate	0.1 in/min
Lead-out Feedrate	0.15 in/min
Ramp Feedrate	0.1 in/min
Plunge Feedrate	0.1 in/min
Maximum Stepdown	0.0689 in
Radial Stock to Leave	0 in
Axial Stock to Leave	0 in

Table B.7: Rough pass speeds and feedrates for a 0.062" 2 flute end mill.

Spindle Speed	8500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	0.1 in/min
Lead-in Feedrate	0.1 in/min
Lead-out Feedrate	0.1 in/min
Ramp Feedrate	0.1 in/min
Plunge Feedrate	0.1 in/min
Maximum Stepdown	0.039 in
Radial Stock to Leave	0 in
Axial Stock to Leave	0 in

Table B.8: Final pass speeds and feedrates for a 0.031" 3 flute end mill.

The following speeds and feedrates are ideal for machining MACOR ceramics with a carbide end mill.

Spindle Speed	9500 rpm
Ramp Spindle Speed	9500 rpm
Cutting Feedrate	0.5 in/min
Lead-in Feedrate	0.2 in/min
Lead-out Feedrate	0.3 in/min
Ramp Feedrate	0.2 in/min
Plunge Feedrate	0.1 in/min
Optimal Load	0.0125 in
Maximum Roughing Stepdown	0.1 in
Radial Stock to Leave	0.02 in
Axial Stock to Leave	0.02 in

Table B.9: Rough pass speeds and feedrates for a 1/8" 2 flute end mill.

The same speeds and feed rates are recommended for the final pass with the four flute end mills for MACOR ceramics.

Appendix C

Piezoelectric Stack Assembly and Wiring

C.1 Materials required

Before starting to assemble the stacks, make sure to have the following items ready:

- 12 EBL#2 piezoelectric shear plates with gold electrode, 0.157 in x 0.157 in x 0.02 in
- 1 copper sheet, 0.15 mm thick
- four sapphire discs, 0.08 in diameter x 0.02 in thickness
- Conductive epoxy, EPO-TEK H21D
- Wire cutter
- Sharp blades
- Tweezers
- Timer
- PID controlled oven

- Sonicator
- Methanol
- Acetone
- Two heavy metal pieces with flat surfaces
- Kim wipes
- Beakers
- Ultrahigh Vacuum (UHV) compatible wire

C.2 Procedure

Before gluing the stacks, the components must be prepared.

- First, cut the copper plates into about 20 0.157 inch squares and a small notch. Then place them in between the two metal plates to flatten them. (Shown in Figure C.1)
- Wipe the piezoelectric shear plates with a Kim wipe and methanol to clean them.
- Mix the two parts of the EPO-TEK H21D epoxy.
- Once the copper squares are flattened, add them to a beaker with acetone and sonicate for about ten minutes. Then, transfer them to a different beaker with methanol and sonicate for about another ten minutes.
- Once the copper squares are done sonicating, we can move on to the stack assembly.

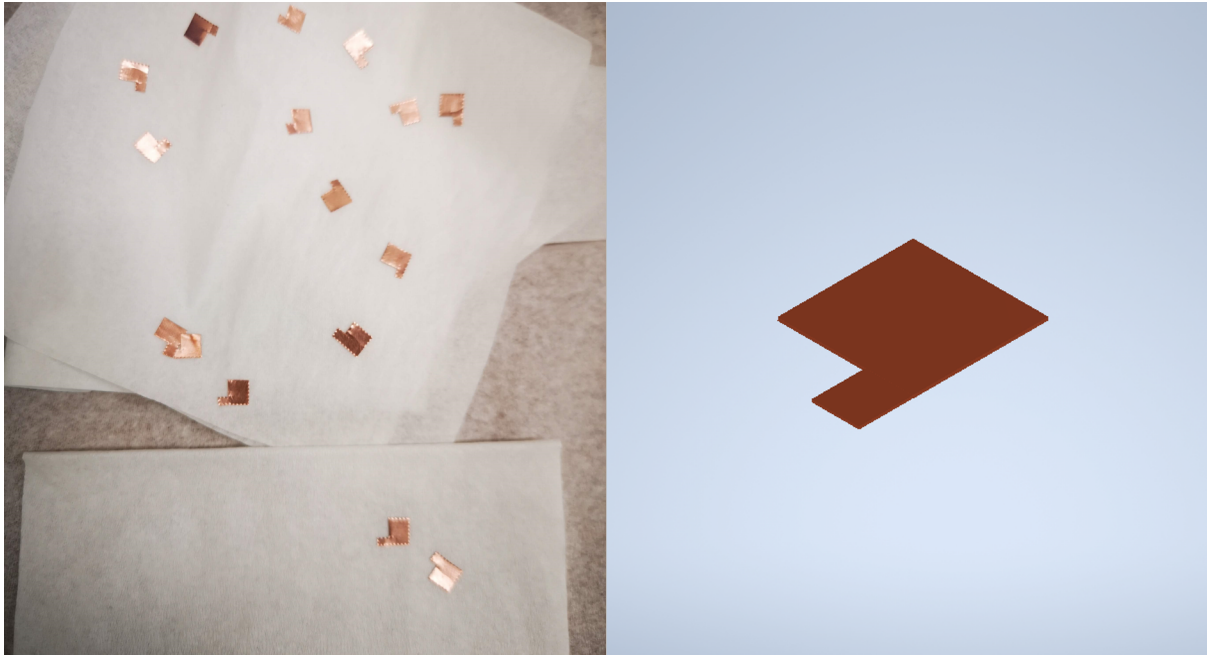


Figure C.1: Copper squares cut from the copper sheet.

The piezoelectric shear plates come with their polarisation directions marked on them. This is very important and needs to be kept in mind while assembling the stacks. The stack assembly procedure is provided below.

- First, preheat the PID (Proportional Integral Derivative) controlled oven to 80°C .
- Follow the procedure shown in Figure C.2 but apply conductive epoxy after each step and bake for about 20 minutes.
- The second piezoelectric shear plate must be flipped upside down and then turned 180 degrees.
- Once the piezoelectric slabs and the copper plates are glued, the sapphire discs can be glued on top of the stack.
- Once the entire stack has been glued following the procedure shown in Figure C.2, the stack can be wired.
- One optional step is to add an alumina slab to the bottom of the stack to prevent any shorts.

- Before wiring, strip the insulating coating on the wire using a sharp blade.
- The wire can be soldered on using UHV-compatible solder or spot welded onto the notch in the copper plates.

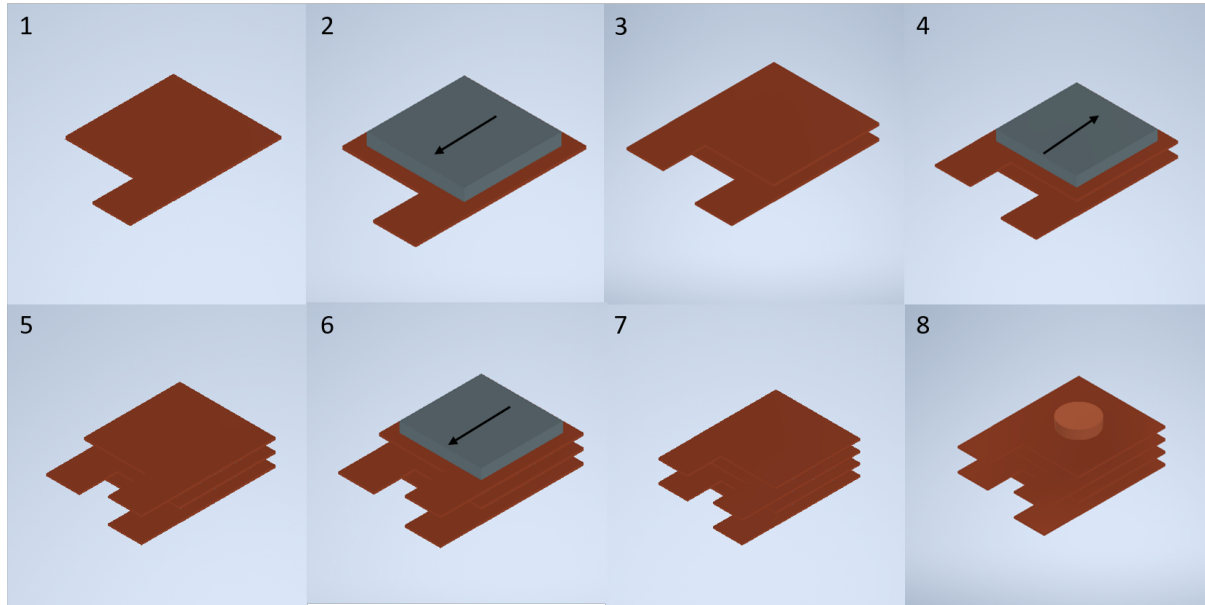


Figure C.2: This is the order and the orientation in which the piezoelectric slabs must be assembled for maximum displacement. The notch position in the copper plates can also be switched to make the wiring process easier and to avoid shorts.

Appendix D

TRUMPF Settings

The following settings were ideal for printing Tekna W-45 powder with a TRUMPF TruPrint 1000 SLM printer. These settings were tried and tested using Materialise Magics slicing software. Ultrahigh pure argon gas is required for the inertization of the build chamber. Oxidization of tungsten powder during the print is a significant problem that needs to be monitored constantly. Proper personal protective equipment must be worn when handling tungsten or any metal powder used for printing, and surfaces must be cleaned thoroughly after working on them with metal powder. Special vacuum cleaners are available to clean metal powder as well.

The following tables provide the Machine Settings in Materialise Magics software for TRUMPF TruPrint 1000 to print tungsten (W). The settings not mentioned in the following tables should be left as the default Refractory Metal settings provided by TRUMPF.

Oxygen Level	0.0100 %
Shielding Gas Speed	2.5 m/s
Shielding Gas Type	Argon
First Layer Iterations	1
Minimum Layer Time	0

Table D.1: Process settings for W with TRUMPF TruPrint 1000.

Delivery	80 mm/s
Application	80 mm/s
Return	250 mm/s

Table D.2: Recoater Speed settings for W with TRUMPF TruPrint 1000.

Dynamic Powder Supply	No
Typical/Maximum Supply Factor	300 %
Supply Factor for First Layers	400 %
Number of First Layers	30
Bulk Density	12.5 kg/dm ³

Table D.3: Powder settings for W with TRUMPF TruPrint 1000.

The build strategy in Materialise Magics should be set to the print settings file provided by TRUMPF for refractory metals.