Practical Implementation of a Physical Vapor Deposition System in a Research Environment

An in-depth look at the implementation of a thermal evaporator system

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Abstract

Even small physical vapor deposition (PVD) systems typically found in research environments can cost hundreds of thousands of dollars, making them unattainable for independent research groups and small startup companies. This work demonstrates the implementation of a low cost thermal evaporation system commissioned for less than \$ 5,000, while maintaining advanced features and capabilities, and not sacrificing functionality. The thermal evaporation system is capable of closed-loop-feedback thickness control of multiple sources, a low-base pressure of $3 \cdot 10^{-7} Torr$, and capable of growing films with resolutions of less then $10nm$. The system is also equipped with an extensive interlock subsystem to protect both the hardware and the user. This document contains a discussion of how each of these capabilities were implemented, along with the obstacles that were overcome.

In addition to the discussion about the thermal evaporator, an introductory overview of other PVD systems such as sputter deposition, electron beam PVD, and pulsed laser deposition is presented. There is also a general discussion about vacuum systems and the relevant physical concepts. Because the PVD systems examined share many attributes, namely aspects of their vacuum system, much of the information covered here can be directly ported to many PVD systems.

Chapter 1

Introduction

This document describes the design, implementation, and characterization of a thermal evaporation system to be put into service for the Materials Synthesis and Characterization faculty and Department of Physics at Oregon State University. It serves as an overview of physical vapor deposition (PVD), with particular attention being paid to the aspects that pertain to the thermal evaporator.

Thin film deposition is the process of depositing materials onto a substrate with thickness ranging less then a nanometer up to several micrometers. The films are typically solid and often referred to as thin solid films. Applications of thin film deposition range from the manufacturing of low tech devices, such as common household mirrors, to cutting edge technologies in the semiconductor, photovoltaic, and optics industries. Thin film deposition falls into two general categories: physical deposition, where films are deposited directly onto a substrate, and chemical deposition, in which the films are formed through chemical reactions. This document discusses physical deposition, more specifically PVD, which is a type of deposition in which the deposited material passes through the vapor phase in order to form the thin film.

PVD processes almost always take place in a vacuum, with the vacuum system being a very important part of the deposition. The vacuum industry has adopted the Torr (sometimes refereed to as millimeter of mercury) as the primary unit of pressure to describe a vacuum. A standard atmosphere is 760 Torr. Vacuums are commonly classified into several categories: low vacuum (atmosphere to 25 Torr), medium vacuum (25 Torr to 1 miliTorr), high vacuum (1 miliTorr to 1 nanoTorr), and ultrahigh vacuum (1 nanoTorr to 1 picoTorr).

Many vacuum systems require two pumps in series because the high vacuum pump must exhaust to a medium vacuum in order to function. In these cases, a medium vacuum pump (medium vac) is used to pump out the foreline (the volume connecting the medium vacuum and high vacuum pumps) to pressures down to the 10s of miliTorr range. A high vacuum pump (high vac) is then used to pump the process chamber to a high vacuum.
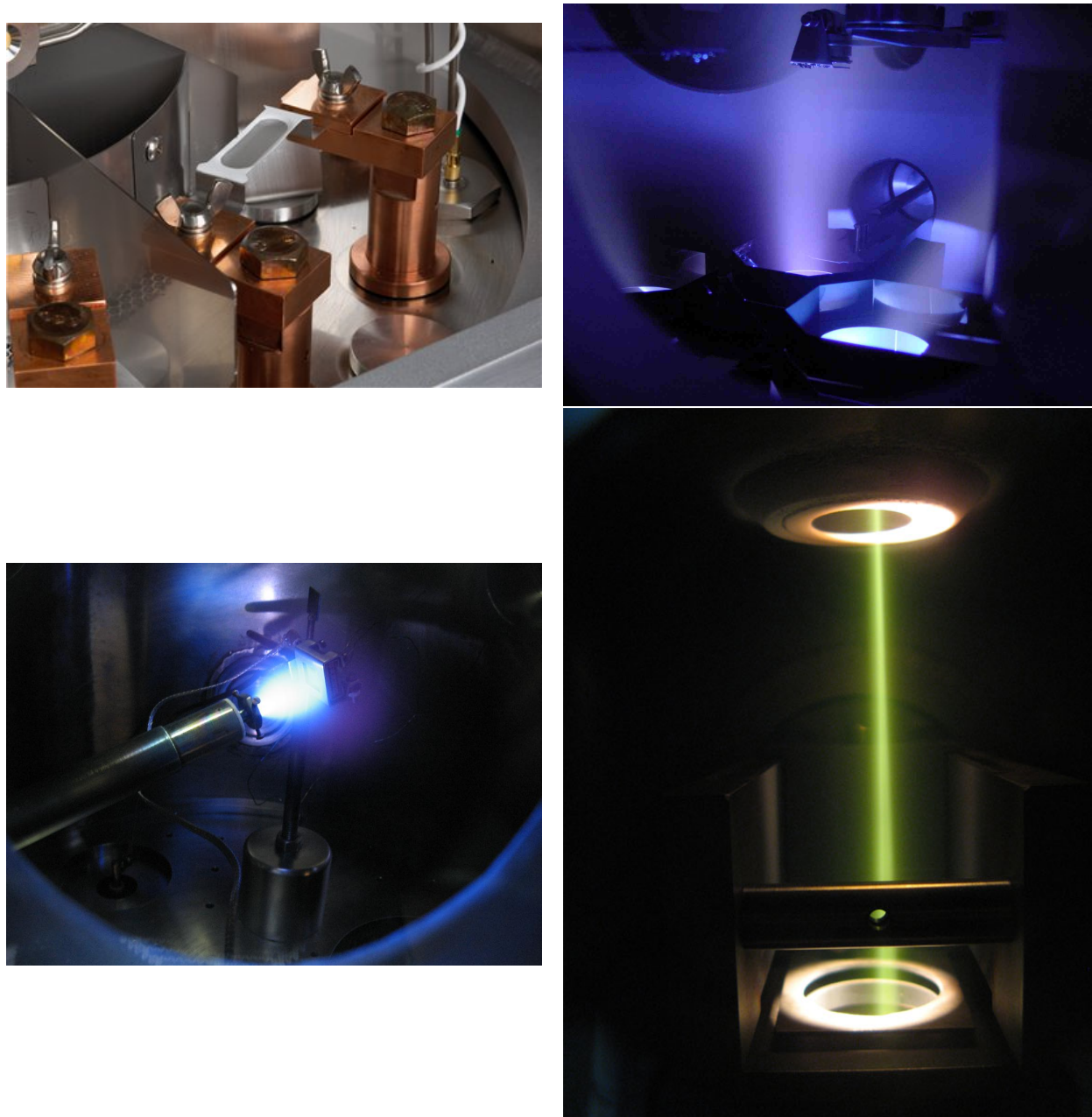
Figure 1.1: **Types of PVD systems.** Upper left: Photograph of thermal evaporation sources. Upper right: Photograph of sputter targets with argon plasma. Lower left: Photograph of a pulsed laser deposition target with vapor plume. Lower right: Photograph of source material being ejected by electron beam in electron beam deposition.

Thermal evaporation is a type of PVD where the deposition material is heated to the point of evaporation, and a substrate is then exposed to the vapor in order to grow a thin film. It is important that the deposition material vapor has a free path to the substrate; this is achieved by conducting the process in a high vacuum.

The free path is quantified by the mean free path Eq. 2.5 which is the average distance that a particle travels, without a measurable interaction with the medium, at a given pressure.

Thermal evaporation takes place at pressures below $10^{-5}Torr$, and as shown in figure 2.3, the mean free path of N_2 is more then 100 m at these pressures. Although it is the mean free path of the source material to nitrogen collision, not a nitrogen to nitrogen collision that is important, the values are still comparable. With the mean free path much greater then the dimensions of a thermal evaporator chamber, there is almost no diffusion in a thermal evaporation process, and the deposition material travels in a straight line from the source to substrate. If a point source and constant rate of evaporation is roughly assumed, the deposition rate of a point on the substrate is proportional to $\frac{1}{r^2}$. This is important when considering the uniformity of the thin film across the substrate.

Chapter 2

Relevant Physics

There are several important physical concepts associated with vacuum systems. Concepts that range between the simple definition of various pressure regimes, to more complex concepts such at the various modes in which vapor moves throughout a vacuum system. A good understanding and strong intuitive model of these concepts is recommended to ensure success while working with vacuum systems.

2.1 Pressure regimes

Pressure is a familiar concept to most, in terms of pressures greater than atmospheric pressure. Typical pressure gauges that are present in everyday life only measure what is referred to as the gauge pressure: the pressure above atmospheric pressure. When dealing with pressures below atmospheric pressure, some new ideas come into play.

Vacuum pressures are divided into four basic regimes. The exact definitions vary, but in modern vacuum applications, *low vacuum* includes pressures between atmosphere (760 Torr) and 25 Torr, *medium vacuum*, between 25 Torr and 1 mTorr, *high vacuum* between 1 mTorr and 1 nTorr, and *ultrahigh vacuum* for pressures less that 1 nTorr.

PVD processes typically take place between medium vacuum and high vacuum. Ultra high vacuum systems are typically analytic systems in which the nature of the measurements they perform require such low pressures.

2.2 Vapor transport in vacuum systems

2.2.1 Diffusion

Diffusion is a mass transport mechanism that describes the process of matter spreading from regions of high concentration to regions of low concentrations. More generally diffusion can also refer to the movement of heat.

Molecules within a fluid are in continuous motion and frequently collide with one another. Because the frequent collisions cause the particles to move in a seemingly random pattern, this motion is referred to as a random walk. To illustrate the concept of diffusion, figure 2.1 shows a computational simulation that tracts the motion of 100 particles undergoing a random walk in an environment comparable to that of a vacuum system. The mean free path of the particles was set to $100mm$, the average velocity was set to $100m/s$, and the time the simulation ran was one second. At the end of the simulation, the average distance from the origin was $4.59m$.
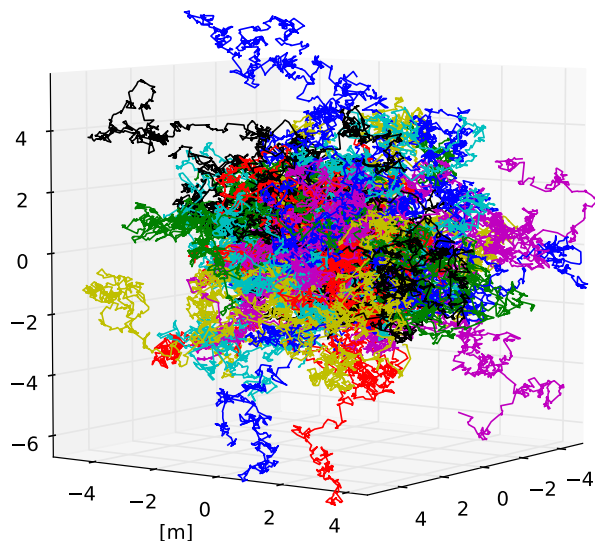
Figure 2.1: A random walk simulation ran for one second of 100 particles starting at the origin.

Performing simulations that model the position of individual particles can only go so far, thus a model to describe diffusion in bulk gas is needed. Maxwell-Stephan diffusion describes the mass (or molar) flux of a gas across a surface. The model states that the flux is proportional to a diffusion coefficient multiplied by

the gradient of the concentration. The general form for the mass flux is given in equation 2.1.

$$J_i = -\rho D_i \nabla c_i \tag{2.1}$$

Where ρ is the density of the gas, D_i is the diffusion coefficient of a particular component of the gas, and c_i is the mass concentration of a particular component of the gas.

The general case can be applied to a component of a gas (a particular substance with in the gas) diffusing through a bulk gas. When considering diffusive flow in regards to a vacuum system, the gas is often considered homogeneous and equation 2.1 reduces to 2.2

$$J = -D \nabla \rho. \tag{2.2}$$

In other words, there is only one component of the gas and the mass flux becomes a function of the density and diffusion coefficient.

Equations 2.1 and 2.2 are referred to as Fick's first law of diffusion. When the time evolution of a system is of interest, Fick's second law of diffusion can be used. For a homogeneous system, the second law is given in equation 2.3.

$$\frac{\partial \rho}{\partial t} = -D(t) \nabla^2 \rho. \tag{2.3}$$

To apply Fick's first and second laws, the diffusion coefficient must be known. The diffusion coefficient is often determined experimentally for a particular situation, but it is also related to the mean free path by the *Einstein-Smoluchowski equation*, equation 2.4.

$$D = \frac{\lambda^2}{2\tau}. \tag{2.4}$$

Where *lambda* is the mean free path, and τ is the average time between collisions.

The mean free path (equation 2.5) is the average distance that a particle will travel, with out a measurable interaction (collision) with the medium.

$$\lambda = \frac{k_b T}{\sqrt{2}\pi d^2 P} \tag{2.5}$$

Where k_b is Boltzmann's constant, T is the temperature in Kelvin, P is the pressure, and πd^2 is the collisional cross section. The collisional cross section is the area of a circle that is formed buy the distance d, which is the sum of the radii of two colliding molecules, as shown in figure 2.2. This, of course, is a simplification assuming that the molecules are spherical and perfectly ridged, but the model works because of the statistical nature of these types of problems where there is approximately uniform probability of scattering in any direction after a collision.
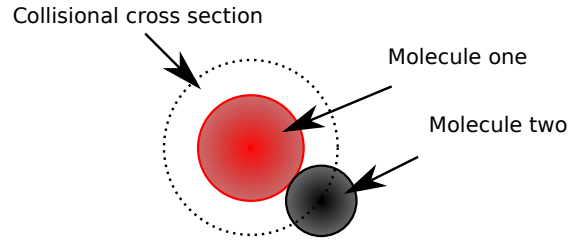
Figure 2.2: The collisional cross section of two molecules defined by the area of a circle with radius equal to the sum of the two radii.

As an example, the average collisional cross section of an N_2 to N_2 collision at room temperature (298.15 K) is about $8 \cdot 10^{-20} m^2$ [2] Figure 2.3 shows the relation of mean free path of diatomic nitrogen to pressure.
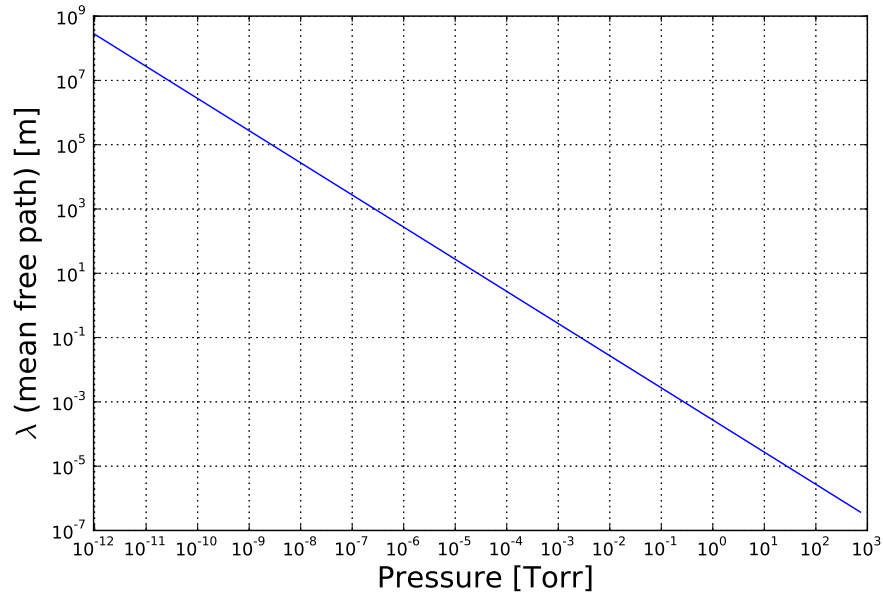
Figure 2.3: The relationship of the mean free path of diatomic nitrogen at room temperature and pressure.

Combining equations 2.4 and 2.5, and relating λ and τ to the average velocity, $(\frac{\lambda}{\tau} = v_{avg})$, the diffusion coefficient can be expressed as in equation 2.6.

$$D = \frac{k_b T v_{avg}}{2\sqrt{2}\pi d^2 P}.$$

(2.6)

Equation 2.7 which is derived from the ideal gas law relates the average speed and temperature.

$$v_{avg} = \sqrt{\frac{3k_b T}{m}}.$$

(2.7)

The final expression for the diffusion coefficient can then be given by equation 2.8

$$D = \frac{k_b T}{2\pi d^2 P} \sqrt{\frac{3k_b T}{2m}}. \tag{2.8}$$

For more reading on diffusion, see [3].

2.2.2 Laminar flow

Some PVD processes flow gas during the deposition, thus laminar flow becomes an important model to understand.

Laminar flow is a fluid dynamics model where the fluid can be thought of as moving in infinitesimally thin layers in which there is no lateral mixing. The flow near surfaces form what is called a boundary layer in which the velocity of the fluid ranges from the free-stream velocity, (v_∞) far from the surface, to zero at the surface. In the simple case (where only one flat surface is considered), the velocity of fluid within each laminar layer is constant. Figure 2.4 depicts the velocity profile near a surface. In the more general case, surfaces and laminar layers can change dramatically, and the velocity of the fluid is not necessarily constant across a laminar layer. However, with a simple application of conservation of mass, it can be shown that the mass flow rate does remain constant.
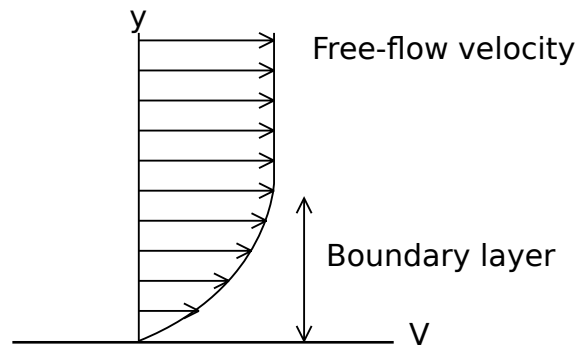
Figure 2.4: Velocity profile of laminar flow near a surface.

The width of the boundary layer (δ) and velocity of a laminar surface are found through an application of Stokes Theorem and depend on shear forces developed between the laminar layers. The resistance to deformation by shear stress is quantified by the viscosity of the fluid.

A useful tool in simplifying calculations is the Reynolds number (Re), defined as the ratio of internal forces to viscous forces. The Reynolds number is given in equation 2.9.

$$Re = \frac{internal forces}{viscous forces} = \frac{\rho L_{char} v_{avg}}{\mu}. \tag{2.9}$$

Where L_{char} is a characteristic length, v_{avg} is the average velocity of the flow and μ is the viscosity of the fluid [5].

The width of the boundary layer of a flat surface can be easily determined using the Reynolds number as shown in equation 2.10.

$$\delta = \frac{5x}{\sqrt{\rho v_\infty x/\mu}} = \frac{5x}{\sqrt{Re}}. \tag{2.10}$$

The x in this case is the characteristic length, or the length from the leading edge along the surface parallel to the flow. δ is defined as the distance from the surface in which the velocity is 99% of v_∞.

2.2.3 Turbulent flow

Turbulent flow is characterized by rapid variations in pressure and velocities in both space and time. The boundary between laminar and turbulent flow is somewhat ambiguous, but it is generally accepted that turbulent flow occurs when the Reynolds number is greater then 5000. Reynolds numbers between 2000 and 4000 are considered to be in the transitional range where well defined models do not exist. [5] Vacuum systems are usually engineered to avoid turbulent flows. However, they still occur in situations such as venting and roughing the chamber and exhaust system.

Analytic solutions to turbulent flows for even the most simple geometry are not possible [5], but useful data is tabulated for many common geometries. An example of this is the Moody chart (figure 2.5), which relates the Reynolds number to the friction factor (f) and relative roughness ($\frac{\epsilon}{D}$) of a circular pipe. The relative roughness is the ratio of the mean surface variation to the diameter of the pipe and the friction factor for a horizontal pipe is given in equation 2.11.

$$f = \frac{2D_h}{L\rho v^2 \Delta P} \tag{2.11}$$

Where D_h is the hydraulic diameter, or simply the diameter of a circular pipe.
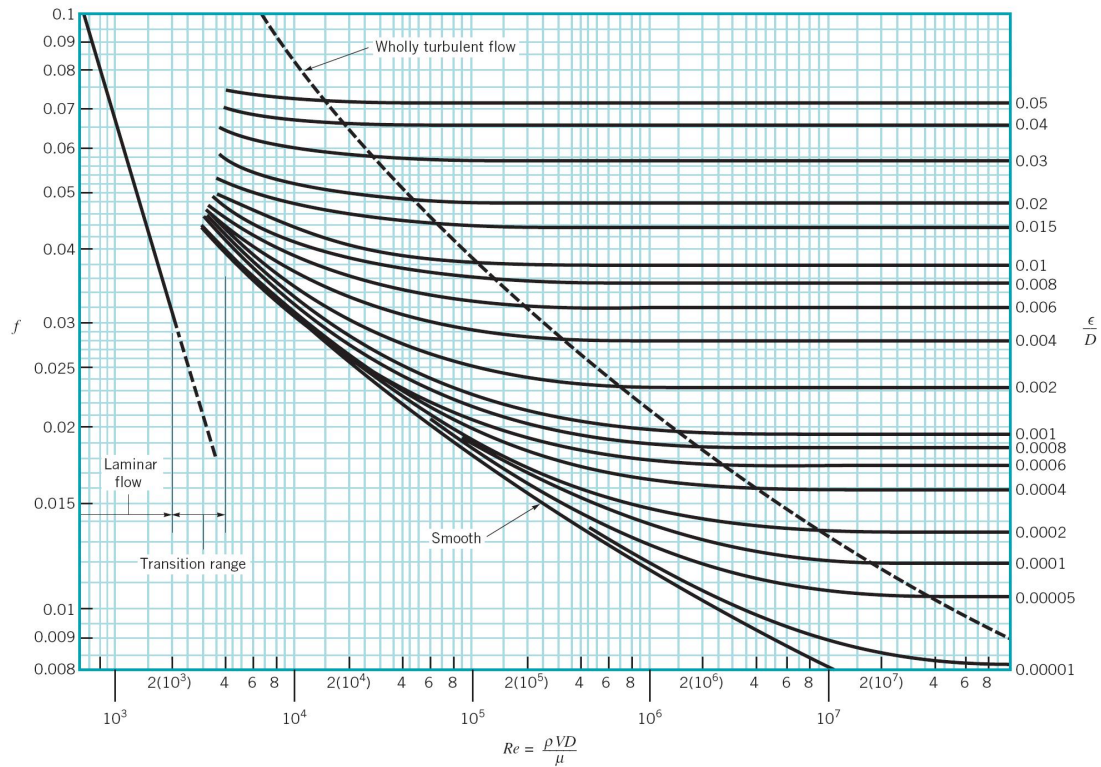
Figure 2.5: Moody Chart: Friction factor as a function of relative roughness and Reynolds number[6].

2.2.4   Critical flow

Critical flow, depicted in figure 2.6, occurs at an orifice when the upstream pressure is much greater than the downstream pressure and the gas reaches sonic velocity. That is, the gas can expand freely from the orifice, at which point the mass flow rate no longer depends on the down stream pressure.

Reducing the downstream pressure typically promotes the flow of a fluid, however a choked plane is formed when the velocity reaches the local sonic velocity. Further reductions in downstream pressure then have no effect on conditions upstream [6].
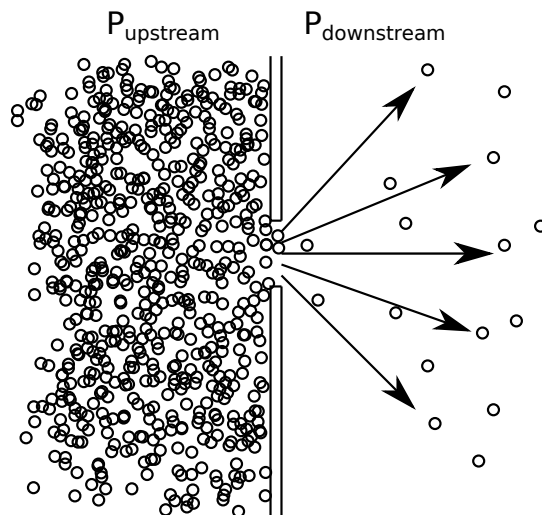
Figure 2.6: Depiction of critical flow at an orifice.

Although critical flow is the extreme case, it is very common in vacuum systems. For instance, when a vacuum chamber is being roughed out, as the roughing valve is first opened critical flow occurs from the chamber, which is at atmosphere, to the medium vacuum pressure at the inlet of the roughing pump. Critical flow also occurs when venting the chamber, indicating that the mass flow rate of vent gas into the chamber is constant until the chamber is near atmospheric pressure. A less dramatic example would be at a small vacuum leak. It is useful to know such situations occur at critical flow because pressure is proportional to the amount of gas in the chamber and at critical flow, the amount of gas crossing the vacuum boundary is constant, thus $\frac{\partial P}{\partial t}$ is constant.

The flow rate can be calculated once it is determined that the velocity of the gas at the orifice is at the sonic velocity in which the condition is given by,

$$\frac{P_u}{P_d} > \left[\frac{2}{(k+1)} \right]^{-k/(k-1)}. \tag{2.12}$$

[6]

Where P_u and P_d are the upstream and downstream pressures respectively, and k is the ratio of specific heat at constant pressure to the specific heat at constant volume, ($k = \frac{c_p}{c_v}$).

After it is determined that the condition in equation 2.12 is met, the critical flow model given by equation 2.13, can be used to determine the mass flow rate.

$$\dot{m} = A \sqrt{ k \rho_u P_u \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} }. \tag{2.13}$$

Where $\dot{m}$ is the mass flow rate, A is the cross-section area of the orifice ($A = \pi D^2/4$ for a circular orifice)

and ρ_u is the upstream density of the gas at a given pressure and temperature. Assuming ideal gas behavior,

$$\rho = \frac{PM}{RT} \tag{2.14}$$

where R is the universal gas constant and M is the molar mass.

Putting it all together, the mass flow rate of a gas as a function of orifice diameter is given by,

$$\dot{m} = \frac{\pi D^2}{4} \sqrt{\frac{kP_u^2M}{RT}\left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}}. \tag{2.15}$$

If the volumetric flow rate is needed, then

$$\dot{V} = \frac{\dot{m}}{\rho_d}. \tag{2.16}$$

Equations 2.15 and 2.16 give the flow rate in Kg/s and m^3/s is SI units. There are two important things to note when performing this calculation. First, although SI units are preferred, the molar mass is often expressed in g/mol and pressure in kPa (kN/m^2), both of which are different by a factor of 1000 from SI units. In this case, the factor of 1000 cancels if both g/mol and kPa are used. It is common practice to use these units but it is important to ensure consistent use. Second, it is important to be aware that the volumetric flow rate is referenced at the downstream pressure in equation 2.16 not upstream, so the density used in that equation is not the same as in equation 2.13.

Flow rates of are often expressed in standard cubic centimeters per minute ($sccm$). To convert to $sccm$, $\dot{V}$ is multiplied by ($[60s/min] \cdot [10^6 cc/m^3]$). In this conversion, the standard pressure and temperature (STP) must be used for the density of the gas, **but not for the temperature**. The temperature is the upstream temperature of the gas, an important parameter in the calculation. The final equation of flow rate measured in $sccm$ is given in equation 2.17.

$$\dot{V}_{sccm} = \frac{\pi \cdot D^2}{4\rho_{stp}} \sqrt{\frac{kP_u^2M}{RT}\left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}} \left[\frac{60s \cdot 10^6 cc}{min \cdot m^3}\right]. \tag{2.17}$$

Chapter 3

Vacuum Systems

Vacuum technology is a vast field. This chapter only serves as a very brief introduction to some aspects of the basic equipment commonly used in vacuum systems. Vacuum systems range in size, between some very small analytic tools in which the vacuum chamber can be measured in cubic centimeters, to integral parts some of the largest machines ever built by humankind. The vacuum system on the Large Hadron Collider at CERN has 54 kms of ultra high vacuum (UHV) to provide a conduit for the collider's particle beam. When including the cryogenic vacuum isolator used to reduce the pressure differential at the UHV interface, the volume of the vacuum exceeds $150,000 m^3$. [7].

3.1 Vacuum Measurements

Conventional pressure gauges work by directly measuring the force applied to a physical barrier separated by a pressure differential. The reference pressure for these types of gauges is usually the ambient atmospheric pressure, meaning they are actually measuring what is known as gauge pressure. At vacuum pressures, it is important to know the absolute pressure. The small forces applied to a surface become much too difficult to measure directly, therefore, other means of measuring pressure are needed.

3.1.1 Thermocouple gauge

Thermocouple gauges work by applying a constant current across a filament with a thermal couple welded to it. The temperature of the filament is primarily dependent on the thermal loss by means of conduction to the system gas. As the pressure drops, the number of gas molecules hitting the filament drops, thereby decreasing the amount of heat carried away from the filament and increasing its temperature. The thermal couple voltage is then mapped directly to pressure in a gauge controller.

The thermal response of the filament to pressure in a typical thermocouple gauge is only measurable between 10 Torr and 1 mTorr. The thermal conductivity depends on the composition of the gas and these types of gauges are typically calibrated for nitrogen. There is a significant deviation of the measured pressure from

the actual pressure, if the composition includes large components of gases other then nitrogen (pressure measurements of air are considered acceptable).

Figure 3.1: Photograph of thermocouple gauge.
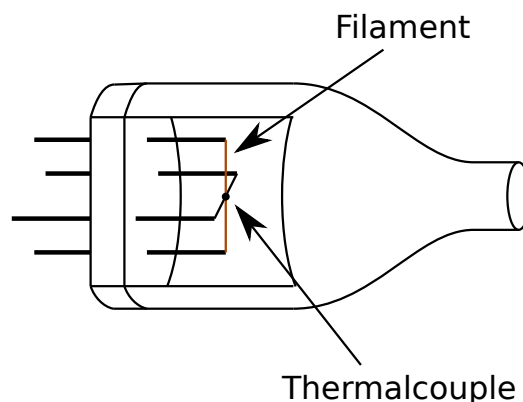
Figure 3.2: Cutaway diagram of a thermocouple gauge.

3.1.2 Convection gauge

Convection gauges are medium to low vacuum pressure gauges that work by measuring heat transport by means of conduction through the gas at low pressures and convection at higher pressures. A convection gauge employs a heated sensing wire that is centered around a temperature compensating winding. The resistance of the wire is temperature dependent, enabling the temperature to be monitored. At low pressures, the convection gauge works in a similar manner to a thermal couple gauge. Heat is transported away from the sensing wire by means of conduction and the rate of heat transfer is dependent on the pressure. Unlike a thermal couple gauge, the convection gauge does not lose sensitivity at higher pressures because it is designed to allow convection currents to develop, enabling an additional mode of heat transport.

Although convection gauges provide a greater range in pressure measurement over thermal couple gauges, there are limitations. In pressure regions where the convection currents become turbulent (above 2 Torr), the response to gas species other then nitrogen becomes non-linear [**Grangville**], and significant deviations in measurements from the true pressure occur. Because the gauge relies on convection currents that carry heat away form the sensor against gravity, the orientation of how that gauge is mounted becomes very important. A convection gauge should always be mounted with the long axis horizontal.

Figure 3.4: Cutaway diagram of a convection gauge.

Figure 3.3: Photograph of convection gauge.

3.1.3 Ionization gauge

An ionization gauge, or more commonly referred to as an ion gauge, is a high vacuum gauge that measures the ionization current from ionized gas in the gauge and a collector. The collector is held at a high potential creating an electric field that accelerates ionized molecules towards it, thereby producing a current. The ionization current is then proportional to the number of ionized molecules that reach the collector. This number depends on the pressure.

There are two main types of ion gauges: hot cathode and cold cathode. Typically, the generic term "ion gauge" refers to a hot cathode ion gauge shown in figure 3.6. This type of ion gauge uses a filament (also the acting cathode) to flood the area with electrons thereby increasing the number of ionized particles and allowing an ionization current to easily develop.

A cold cathode ion gauge, or Penning gauge, does not have a filament. Instead, it uses a greater potential (around 2kV) and relies on an avalanche effect, where one ionization event produces additional charge carriers that can gain enough energy to cause other ionization events. Permanent magnets are used to cause the electrons to move in a helical motion, increasing both the path length, and chance of causing additional ionization events. At low pressures, it becomes difficult to initiate an ionization current. Another disadvantage is that the energies of the ionized species are large enough to cause sputtering at the anode and pollute the vacuum system [4].

Figure 3.5: Photograph of an ion gauge.
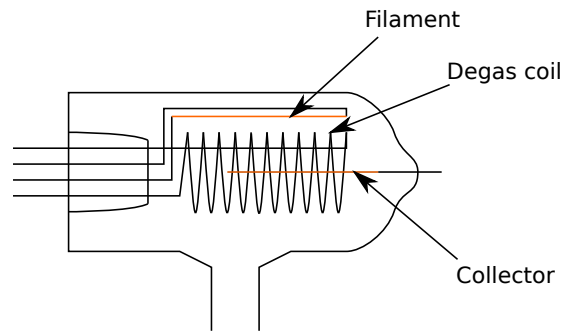
Figure 3.6: Diagram of an ion gauge.

3.2   Vacuum Pumps

There are many types of vacuum pumps that excel in particular applications. For typical vacuum systems, there are two main categories that vacuum pumps fall under: medium and high vacuum pumps. Systems capable of high vacuum almost always have pumps in both categories for two reasons. First, a true high vacuum pump cannot operate at pressures near atmosphere. A medium vacuum pump is required for a process known as roughing the chamber, which means to pump the vacuum chamber down to a pressure that the high vacuum pump can operate. Safe cross over pressures vary from pump to pump, but typical values range between 10 and 100 mTorr. The second reason both medium and high vacuum pumps are required in high vacuum systems is that most high vacuum pumps cannot exhaust to atmosphere. A medium vacuum pump is hooked up in series to provide an appropriate backing pressure backing pressure, that without could result in severe damage to the high vacuum pump.

3.2.1   Medium Vacuum Pumps

Commonly referred to as mechanical pumps, medium vacuum pumps, as the name implies, have base inlet pressure in the medium vacuum regime. Historically, high vacuum pumps did not have any moving parts, so a mechanical pump was an appropriate name to describe pumps such as rotary vane or piston pumps. Figure 3.7 shows the basic pumping operation of a rotary vane medium vacuum pump.
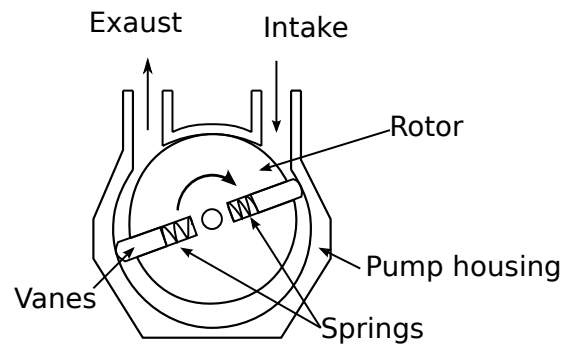
Figure 3.7: Diagram of a rotary vane mechanical pump.

3.2.2 Diffusion Pump

A diffusion pump is a high vacuum pump that has no moving parts and works by heating oil and channeling the vapor in a downward direction, as shown in figure 3.8. The oil jets then either capture or transfer momentum to gas causing a downward flow and pressure differential. The sides of a diffusion pump are cooled to bring the energy of the oil and captured gas down, and mitigate back-streaming.
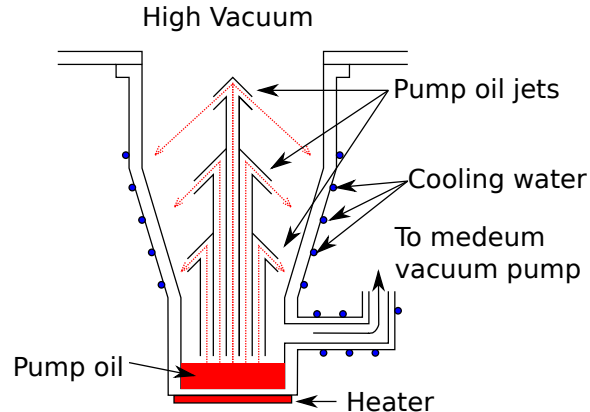
Figure 3.8: Diagram of a diffusion pump.

A diffusion pump must be backed by a medium vacuum pump to maintain a pressure at the base that is low enough to effectively pump, and prevent stress on the oil. If the backing pressure is too high, the oil does not evaporate as quickly causing it to overheat. Also, a higher pressure means that there is also more oxygen and the oil burns which can destroy a pump.

Another aspect to be aware of is the process byproducts and how their effect on the pump oil.

3.2.3 Turbo Molecular Pump

A turbo molecular, or just turbo pump, is a high vacuum pump that has a stator and rotor with several stages of blades that simply transfer the momentum of vapor driving it toward lower stages. The vapor is then exhausted through the foreline, which is backed by a medium vacuum pump. Notice the decrease in the pitch of the blades in the lower stages in figure 3.9.

Figure 3.9: Photograph of a turbo pump with cut out showing the stator and rotor.

Like the diffusion pump, the turbo pump must be backed by a medium vacuum pump. A typical rotation speed for a turbo pump is about 30,000 rpms, and if the backing pressure rises too high, it will increase the load on the motor to a point it is not designed to handle. Reactive process byproducts can also damage a turbo pump. The bearings are particularly at risk. Damage can be mitigated by flowing inert gas over the bearings while processing. Some turbo pumps have magnetically levitated bearings which further increase the resistance to stress caused from process byproducts.

Chapter 4

Thermal Evaporation

A common PVD method of creating thin films is thermal evaporation. With thermal evaporation, the deposition material (source) is heated to the point of evaporation in a high vacuum and the vapor is exposed to the substrate in order to grow a thin film.

The source is heated by means of Ohmic resistance through a boat that is a specially designed heating element. To avoid contamination of the thin film, the boat must be made with refractory metals such as tungsten, molybdenum, and tantalum, or alloys thereof. Refractory metals are heat resistant in the sense that they have high melting points and enthalpy of vaporizations, critical characteristics of a thermal evaporation boat.

The deposition process is controlled by regulating the current driven through the boat and comparing it to feedback from a crystal thickness monitor. This can be done manually or with a closed loop control circuit.

A crystal thickness monitor can measure the thickness and rate of deposition of a thin film while it is being deposited. A crystal thickness monitor works by using a quartz crystal microbalance (QCM), in which vibrations in the crystal cause the stress to oscillate at the mechanical resonance of the particular crystal used. Because quartz is a piezoelectric material, the oscillating stress causes an oscillating electric charge, which produces a measurable signal. This signal is used to measure the rate of mass deposited on the quartz resonator by evaluating the change in the mechanical resonance of the crystal. As mass is deposited on the crystal, the mechanical resonance is decreased by an amount roughly proportional to the mass per unit area of the deposited film. If the density of the film is known, the thickness can be determined.

Because the process takes place in a high vacuum, the source vapor travels in a straight line. This allows for the rate of deposition at any given point to have a simple geometric relation to the location of the source. For instance, if a point source is assumed, the deposition rate at any given point on a surface is given by

$$\rho = \frac{E}{r^2}. \tag{4.1}$$

Where ρ is the rate of deposition at a given point on a surface, and E is the rate of evaporation at the source.

When starting the evaporation, the substrate is shielded from the source by a shutter, while the thickness monitor remains exposed. Once an appropriate deposition rate (usually in the angstroms per second scale) is achieved via the control sequence, the shutter is opened to expose the substrate to the source. When the desired thickness of the thin film is reached, the shutter is closed and the evaporation is stopped.

With a constant rate of evaporation, the deposition rate has a $\frac{1}{r^2}$ dependence, as seen in equation 4.1. This is important when considering the uniformity of the thin film across the substrate. Once the rate of deposition is determined at the thickness monitor, E can be determined and the rate of deposition across the substrate follows.

Tolerable uniformity is typically achieved by making the distance r large compared to the distance across the substrate. In research settings, the substrate is usually small (25x25 mm square slides are common). For example, the thickness uniformity across a 25 mm square substrate, centered over the source at a distance of 0.25 m, is given by

Figure 4.1: The geometry of an evaporation.

$$\frac{\rho_2}{\rho_1} = \left(\frac{r_1}{r_2}\right)^2 = \frac{(0.25m)^2}{(0.25m)^2 + \left(\frac{\sqrt{2} \cdot 0.025m}{2}\right)} \approx 0.998, \qquad (4.2)$$

or about 99.8% uniformity across the substrate.

In commercial applications where the substrates can be up to 450 mm in diameter, there are economic constraints that prevent increasing the distance from the source to the substrate to achieve tolerable uniformities. A large distance between the source and substrate gives rise to several issues, namely, more source material is wasted. This can be costly, especially for materials such as gold or platinum. Also, the physical dimensions of the vacuum system play a huge role in the initial cost and cost of maintenance of the vacuum system. These issues are mitigated by introducing mechanical arrays that rotate and translate the substrate or source in such a way to achieve tolerable uniformity.

Substrate

Deposition
material in
vapor phase

To high vacuum
pump

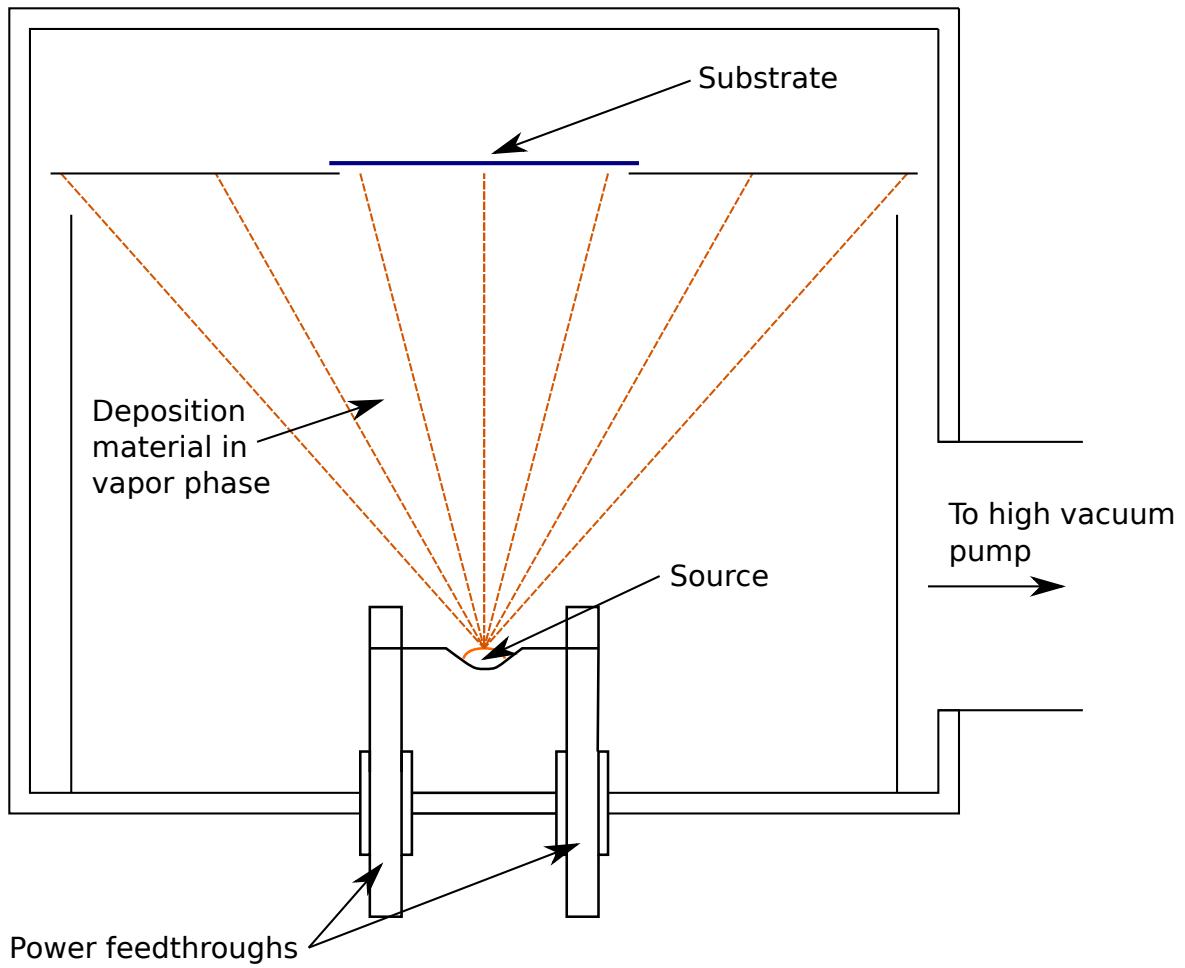Source

Power feedthroughs

Figure 4.2: Diagram of a thermal evaporation deposition process.

Chapter 5

Thermal Evaporation Project

Figure 5.1: Photograph of the Schrader Thermal Evaporation System taken in June of 2012.

5.1 Motivation

The project started in the Spring of 2012 when Janet Tate, a professor of physics at Oregon State University, showed interest in bringing an old thermal evaporator built by Schrader Vacuum Company into service. The original system was a stainless steel evaporation chamber with a rotary vane roughing pump, and a cryopump for high vacuum. The system had been out of service as a true thermal evaporator for several years due to the cryopump failing. However, the chamber was still being used to provide a controlled environment to perform experiments in the medium vacuum to atmospheric pressure range.

Chris Tasker, the development engineer for the Department of Electrical Engineering and Computer Science (EECS) at Oregon State University, accepted the project as part of the Materials Synthesis and Characterization (MaSC) initiative. Dr. Tate is a member of the MaSC faculty who are a group of faculty members whose research is related to material science. The primary purpose of the group is to provide a collaborative environment amongst researchers in various departments, and extend the infrastructure available to the faculty members and their students. Currently, MaSC faculty includes professors of physics, chemistry, electrical engineering, mechanical engineering, and chemical engineering.

Mr. Tasker is the key member of the support staff for MaSC. I work for EECS as a research assistant, however, I am also a student in physics. This further motivated the project and Mr. Tasker ultimately tasked me to rebuild the Schrader system in Professor Tate's laboratory.

5.2 Design and Construction

5.2.1 Initial considerations

Part of the MaSC initiative is to provide a more extensive infrastructure with a reduced overhead through collaboration between departments, rather than having each department fend for itself. The thermal evaporator project provided an opportunity to demonstrate this paradigm by designing and constructing a functioning thin film deposition system, using almost exclusively parts on hand, salvaged from various decommissioned systems that may have otherwise gone to surplus.

Of the original system, the only parts that could be successfully preserved were the chamber, chassis, and a few valves.[1] The first task was to determine if the project was feasible.

The entire system is built around the chamber. Naturally, the chamber needed to be thoroughly inspected. All the flanges are conflat, which are rated for ultra high vacuum, and when installed properly, they are extremely reliable. On the other hand, the door, which is about $400x500mm$, was o-ring sealed. This is not ideal in a high vacuum system because even a small deformation in the chamber, hinges (which are welded to the chamber preventing the opportunity for adjustment), or a small abrasion on the sealing surface could cause the chamber to have a difficult-to-repair leak.

---

[1]The roughing pump of the original system (or medium vacuum pump in the context of the new system) was initially preserved, but do to an abnormal noise, subpar performance, and the cost of repairs, that pump was later replaced.

5.2.2   Leak detection

An important concept to have when leak checking is that everything leaks; it is just a question of the rate at which it is leaking[1].

To check the chamber for leaks, a Varian Mass Spectrometer helium leak detector was used (figure 5.2). This type of leak detector consists of a medium vacuum pump, a high vacuum pump, a valve control network, and a mass spectrometer designed specifically for the detection of helium.

The leak checker has two modes of operation. In the first mode, the test object is filled with helium, and a "snooper" (which is just a needle like nozzle with a known leak rate on a vacuum hose) is attached to the leak detector. The snooper is then moved around the test object, "snooping" for leaks. In the second mode, the leak detector is attached directly to the test object which is pumped down to a medium vacuum. Helium is then applied to the exterior of the test object in areas in which a leak may exist.

The leak detector works by pumping a volume, whether it be a snooper or the test object, down to a safe backing pressure for the turbo pump (usually below 100 mTorr). The turbo pump and mass spectrometer are isolated while the test volume is roughing, so care must be taken to ensure the backing pressure does not raise too high. Although the backing pressure cannot be monitored directly the pressure in the mass spectrometer gives an indication of what it is. The pressure differential across the turbo pump is approximately constant over its normal operating range, so as the backing pressure increases, the pressure in the mass spectrometer also increases. On this particular model of leak detectors, the safe pressure range for the mass spectrometer is clearly marked with a green band on the filament pressure gauge.

Figure 5.2: Varian model 938, Mass Spectrometer helium leak detector.

Once the test volume is roughed out, the turbo pump's *backing line* (what is normally considered the foreline), is opened to the test volume. Notice that this is a stark contrast to the normal operation of a vacuum system, but that is the key to how the leak detector works.

The only volume that the turbo pump is working on it the mass spectrometer This means that in order for a leak to be detected, gas escaping from a leak must travel backwards through the turbo pump to make it to the mass spectrometer This is why helium is used. He_2 being a light molecule travels much faster at the same temperature then the nitrogen and oxygen that make up most of air. Where most gas is blocked by the turbo pump, helium is able to pass though with ease and be detected by the mass spectrometer.

In the case of the Schrader chamber, the leak detector was used in the second mode of operation where the entire chamber was roughed out to preform the leak detection. To do this, first all the major components needed to be removed and of the flanges blanked. This was mainly the high vacuum gate valve that isolates the chamber from the high vacuum pump. Unless these types of gate valves, which are pneumatically operated, are supplied with compressed gas, the valve is in an indeterminate state and therefore needed

to be removed from the chamber to preform the initial leak check. The sealing surface for the o-ring was thoroughly cleaned, along with the o-ring itself. o-ring seals, or any soft seals, are common places to find leaks on vacuum systems such as this one.

In the first check, the leak detector cold not pump the chamber down far enough (below 100 mTorr) to operate. This was an indication that there was a large leak somewhere in either the chamber or the plumbing connecting the leak detector to the chamber.

It is important to note that a "large leak" is a relative term. There is a wide range where a leak may be to large to detect with a leak detector, but much too small to detect by traditional means (soap bubbles). Therefore, through a process of elimination, suspicious components were removed and the flanges were blanked until the pressure could become low enough to operate the leak detector.

With the leak detector, numerous other leaks were found, but all of which were easily repaired by either removing a component and blanking the flange, or replacing a gasket (or o-ring in the case of the hatch which was leaking in four locations).

5.2.3 Other feasibility considerations

Once the chamber was certifiably leak tight, the next step was to procure the components for the vacuum system. There was a turbo pump from a sputter system that had been out of service for several years that was available for use on the evaporator. The turbo pump had the correct sized flange (10" conflat) and was in remarkably good condition. However, the chassis of the evaporator was not designed to support it.

Significant modifications to the frame were required for the chassis to be able to accept the turbo pump. There was a vertical support member that made it impossible to mount the turbo pump. Also, after careful measurements of the physical dimensions of the turbo pump, it was determined that even with the modifications, there was still only about 1 mm of tolerance for the pump to fit within the frame, and only if the pump was positioned in a specific orientation. A redesign and reconstruction of the entire chassis would be required to increase that tolerance by an appreciable amount. After some deliberating on the matter (and a little persuasion), it was decided that even though it was a very tight fit, it was still feasible to integrate that particular turbo pump and the decision was made to move forward with the project by removing the vertical support member and replacing it by a much stronger horizontal cross-member as shown in figures 5.3 and 5.4.
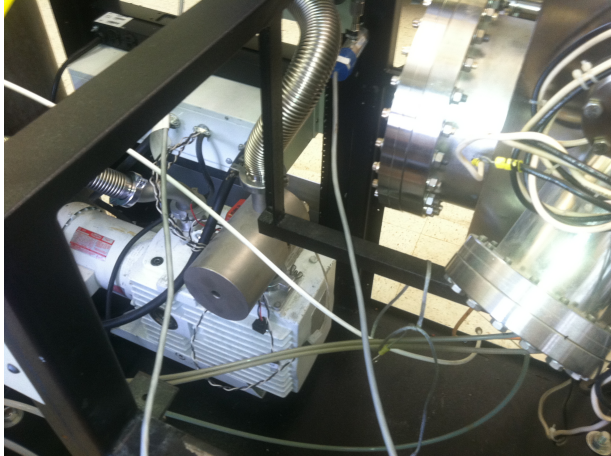
Figure 5.3: A photograph of the internal framework of the evaporator chassis *before* the modifications to the frame. The vertical support member in the center of the chassis prevented the turbo pump from being able to fit on the 10" flange.
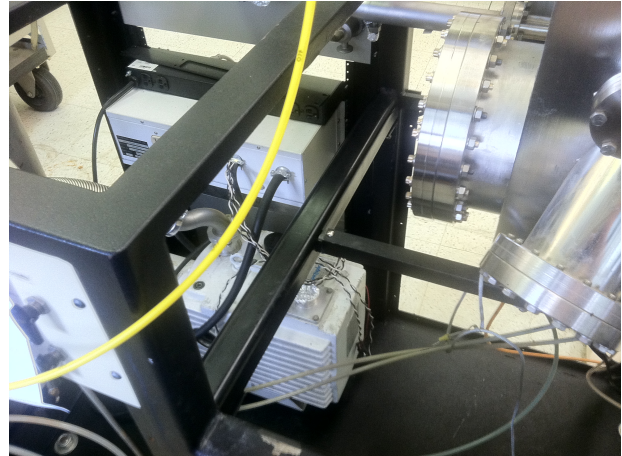

Figure 5.4: A photograph of the internal framework of the evaporator chassis *after* the modifications to the frame. The $1mm$ tolerance referred to in the text is at the bottom face of the upper horizontal cross member.

The next step in the process was to put together the vacuum system. There are significant differences between the cryopump vacuum system and the new turbo pump system that was being implemented. Other than the most obvious difference of the two systems – having completely different types of high vacuum pumps – the difference in operation requirements of the two types of pumps put new constraints on the system and required a complete redesign of the vacuum system layout.

5.2.4 Safety considerations

Two types of safety must be considered in the design/implementation of a system such as the Schrader: the safety of the user and the safety of the machine. User safety is obviously the most important and should be continuously considered at every stage in the design process. With each additional feature added, how user safety is affected should be given serious consideration, no matter how trivial it may seem. It should also never be assumed that the user will use the system as intended and ensure there are reasonable safeguards implemented to account for any foreseeable scenarios.

With the evaporator system, some of the primary hazards to the user include: electric shock, moving parts of the medium vacuum pump, mechanical failure, and many more. The designers can take steps to mitigate many of the hazards associated with this type of system.

It is important that appropriate guards are installed that cover any exposed electric contacts and moving parts. The original evaporator system had a fairly robust set of covers to protect the user. Unfortunately, there were modifications to the system that prevented some of the original covers from being used.

An example of this is the current drive for the evaporation system. It was not a standard 19" rack mount, so it was mounted in place of one of the guards. Fortunately, the person who added it did not put it in the front. Though that would have been the most convenient, it would have also left the largest portion of

the system exposed. The current drive happens to be one of the more hazardous components on the system because of the exposed 208 V electrodes on the back, making it important that guards be put in place.

At the time, the three channel current drive on the system was not working. To keep the project moving, it was temporarily replaced with a simple but reliable variable transformer. The variable transformer was mounted on a panel with the same dimensions of the current drive for easy reimplementation once the three channel current drive was repaired. To make the setup more convenient for the user, current drive was relocated to the front of the system. The front cover was modified such that both it and the current drive could still be installed, ensuring all exposed electrodes were properly guarded.

5.2.5   Protecting the equipment and the interlock system

Because we live at atmospheric pressure (about 760 Torr), the amount of force exerted by it is easily overlooked. A quick calculation of the force exerted by atmosphere on a tangible part of a vacuum system is often used to help people gain perspective. For example, the door on the thermal evaporator is roughly 1/2 of a meter wide, by 3/4 of a meter tall, or $0.375m^2$. Atmospheric pressure is about 100 kPa, or 100,000 N/m. Therefore, when the system is under vacuum, the force from atmospheric pressure on the door is

$$100,000 N/m \cdot 0.375m = 37,500 N, \tag{5.1}$$

more than enough to lift a large sports utility vehicle.

Equipment on systems that operate at high vacuum is very sensitive to pressure can be easily damaged and is expensive to repair or replace. The turbo pump for example must be maintained at a low backing pressure or serious damage will occur. Under no circumstances can it ever be exposed to atmosphere while operational. If exposure occurs, the results would be catastrophic.

Among other things, interlock systems help protect the equipment from sudden changes in pressure. They ensure that the system is relatively safe, if an error is made by a user, or if there is a power failure. Although many sophisticated interlock systems are controlled by computers, it is important to have a basic functionality hardwired. This ensure that, in the event of a power or computer failure, the system will automatically move into a safe state.

The evaporator system has two important volumes in which the pressure is critical. The first is the chamber. The chamber is continuously monitored by a convection gauge, part of the interlock circuit. The gauge controller has a normally open relay that is only closed when the pressure is below a set point. This relay is connected to another normally open relay that supplies power to the high vacuum valve and current sources. This ensures that the high vacuum valve cannot be opened and the current drives cannot be used unless the pressure is at a safe level. It also ensures that if the pressure rises too high while the high vacuum valve is opened, it closes immediately.

The second important pressure is the foreline, or backing pressure. The foreline connects directly to the turbo pump and provides a path from the turbo pump exhaust to the medium vacuum pump. A second convection gauge is connected to the foreline and a similar setup to the interlock is used for the chamber

pressure. The difference is, that if the foreline interlock is tripped, all isolation valves are closed and the whole system is shutdown. The same thing happens in the event of a power failure. Figure 5.5
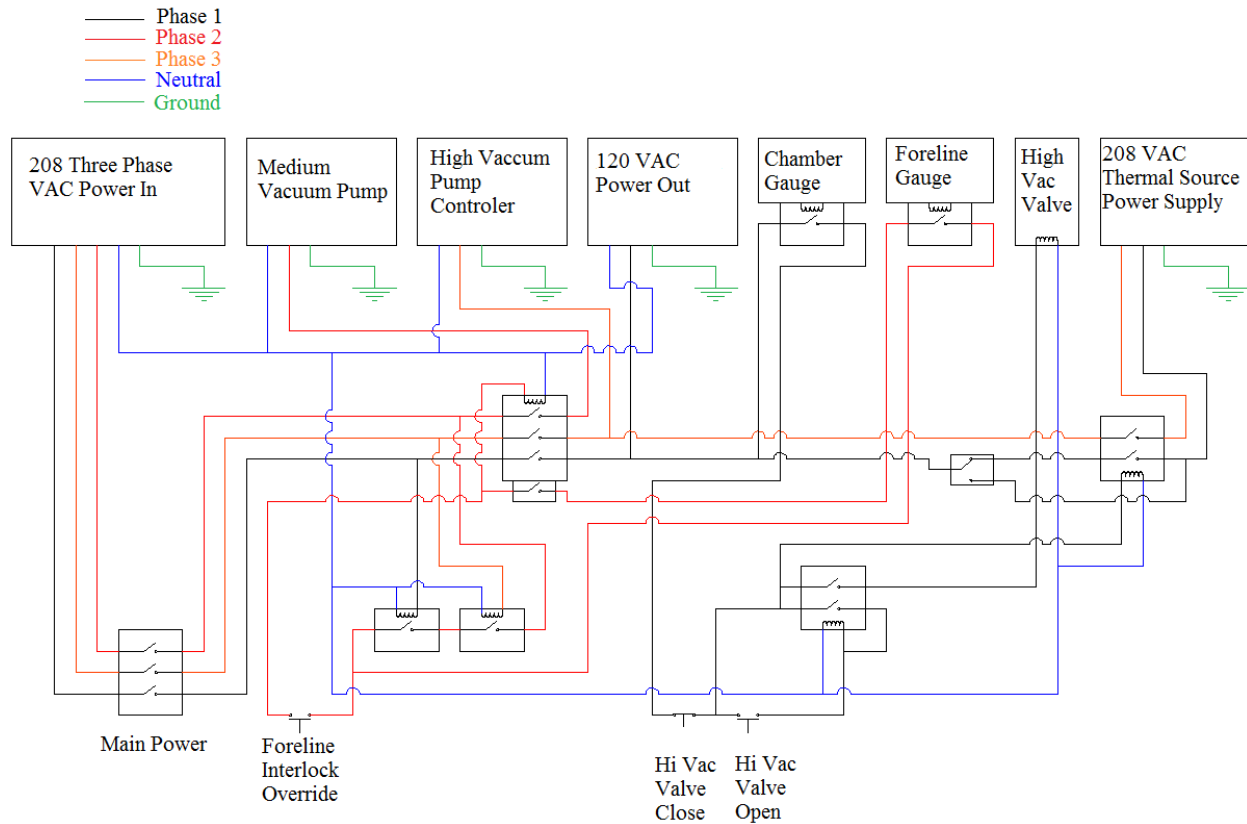
Figure 5.5: Diagram of the interlock system.

5.2.6 The current state of the project

As a thermal evaporator, the system is in service. The chamber base pressure is $3 \cdot 10^{-7} Torr$ and in preliminary tests, the system was able to grow an aluminum film of less then 10 nm. Figure 5.6 is a diagram of the main components of the system as it stands as of the writing of this document. There are talks of implementing upgrades to the system, such as a load lock, and integrating sputtering capability.
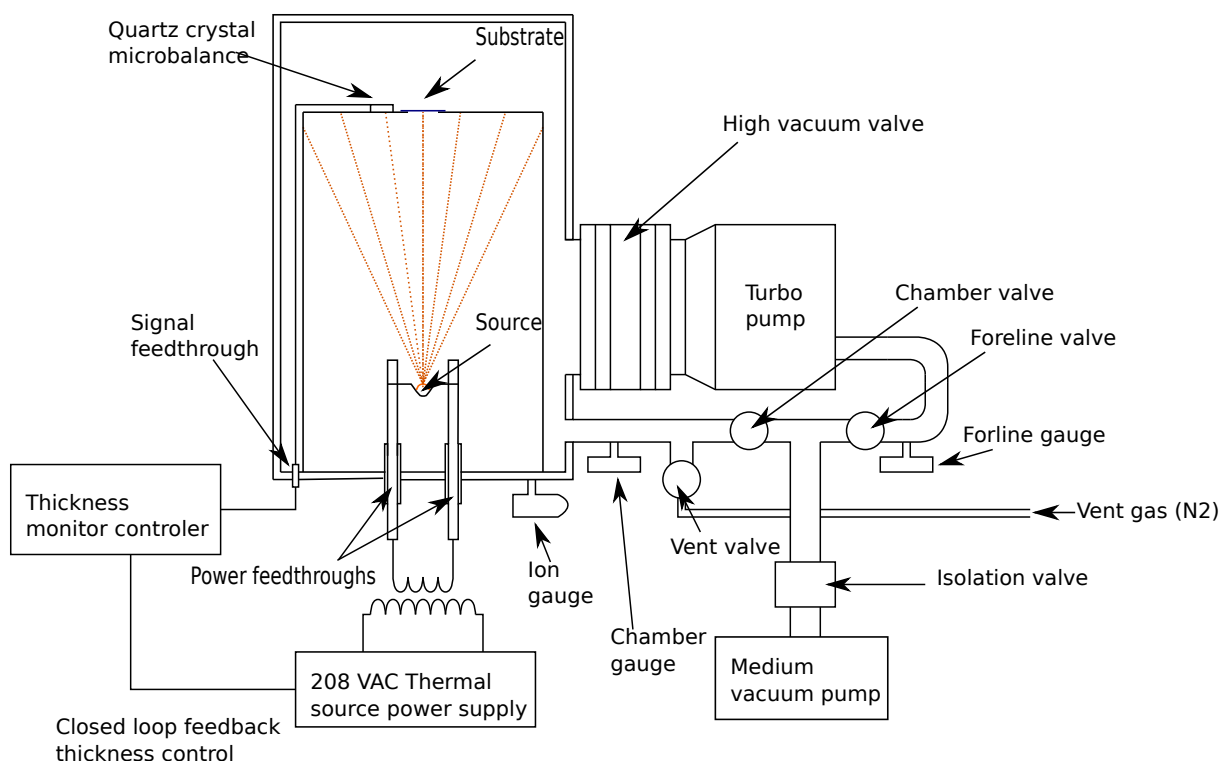
Figure 5.6: Diagram of the thermal evaporation system.

The way the setup works now, the chamber must be vented before and after each use. By doing so, a large amount of gas is absorbed into all the surfaces in the chamber. It takes about an hour to pump the chamber back down to a pressure where a thermal evaporation can be conducted (usually below $10^{-5}Torr$). The time requirement is primarily due to the time required for everything that was exposed to atmosphere to outgas.

A load lock would significantly reduce the time required to set up an evaporation by not exposing the chamber to atmosphere. Only the small volume of the load lock, which is kept immaculate to minimize absorption, is ever exposed to atmosphere.

Another way to reduce the lead time would be to thoroughly clean the chamber and make sure that the shielding is always properly used. On the original system, there was no shielding. Over time, the chamber walls were coated with the films of every deposition ever performed in the tool. Outgassing is particularly slow when there are many layers of material where gas can be trapped. Ideally, the chamber would be electropolished to minimize the surface area, and therefore minimizing the pump down speed, but a thorough cleaning with absolutely nothing abrasive, would go a long way.

This project demonstrated that a useful tool can be put into service without spending a lot of money. The majority of the resources that went into this project was the time spent developing and assembling. With only a few exceptions, the parts used in this project were all parts that were on hand, and would likely not get used otherwise. As with most research tools, there is always more work that could be done to improve the system, but having a working tool rather then a store room full of parts, only adds to the infrastructure

available to the faculty and students.

Bibliography

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[2] P G Brooker and J D E Beynon. "The determination of the collision cross section for momentum transfer of nitrogen by two different experimental techniques". In: *Journal of Physics B: Atomic and Molecular Physics* 5.6 (1972).

[3] Cliford Ho and Stephen Webb. *Gas Transport in Porous Media.* Springer, 2006.

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[5] Deborah Kaminski and Michael Jensen. *Intoduction to Thermal and Fluids Engineering.* 2005.

[6] B R. Munson, D.F. Young, and T.H. Okiishi. *Fundamentals of Fluid Mechanics.* 4th. John Wiley and Sons, 2002.

[7] *Proc. Proceedings of EPAC08, Genoa, Italy.* Accelerator Technology. CERN, Geneva, Switzerland: Vacuum Technology, 2008.

Appendix A

Schrader Manual

A.1   Vacuum system description and nomenclature

Chamber: 16 x 16 x 20 inch stainless steel box with multiple Conflat flanges and a full opining door that is o-ring sealed.

Medium Vacuum Pump: Welch model 1397 DuoSeal belt drive rotary vane mechanical pump, referred to in this manual as the medium vac pump.

High Vacuum Pump: Varian TV 1000 turbo molecular pump, referred to in this manual as the turbo pump.

Foreline: 40 mm stainless steel flex hose connecting the turbo pump to the medium vac junction, the foreline is isolated from the medium vac pump by means of the foreline valve.

Medium Vac Junction: Connects the medium vac pump to the foreline valve and roughing valve.

Foreline Valve: Manually operated poppet valve, connecting the foreline to the medium vac junction.

Roughing Valve: Manually operated poppet valve, connecting the chamber to the medium vac junction.

Vent Valve: Manually operated poppet valve, connecting the chamber to a low pressure dry nitrogen source.

Hi Vac Valve: Electronically controlled, pneumatically operated, 10 inch Conflat gate valve, connecting the turbo pump to the chamber.

Foreline and Chamber Pressure Gauges: Granville Phillips Convectron gauges with 275 analog Convectron gauge controllers.

Ion Gauge: Tungsten filament ion gauge connected to the chamber used to measure hi vacuum pressures (below 10^{-4} torr).

Medium Vac Pump Isolation Valve: An electromechanical valve that will close upon a power failure or interlock activation. This valve prevents back streaming of pump oil, and contamination of the vacuum system.

A.2 Utilities

AC Power: The system has a single point electrical power connection that requires three-phase 208 volt AC power.

Pneumatic Actuation Gas: The operation of the hi-vac valve requires either compressed air or nitrogen between 70 and 80 psi, supplied to the Swagelok connection labeled compressed air on the back side of the machine.

Vent Gas: Dry nitrogen at no more than 5 psi should be supplied to the Swagelok connector labeled "Vent Nitrogen" on the back side of the machine.

Cooling Water: The thickness monitors require cooling water in which the supply and return for is located on the back of the machine.

A.3 Vacuum System Operating Procedures

A.3.1 System start up procedure

This section outlines the procedure for starting the vacuum system from an unknown state.

1. Check the actuation nitrogen, or compressed air supply, and ensure that the tank valve is fully opened and the pressure on the downstream side of the regulator is between 70 and 80 psi.

2. Ensure all valves on the front panel are closed.

   Note: The foreline valve may be open if there was a power failure, or the machine was shutdown improperly. The foreline valve should be closed on start-up to prevent back streaming of medium vac pump oil.

3. Switch the main power breaker to the on position. The main power indicator light should be lit.

4. Press and hold the foreline interlock override button, the medium vac pump should start.

   Note: The turbo pump may try and start if there was a power failure or the machine was shut down improperly. If this happens, press the start/stop button on the turbo pump controller.

5. While holding the foreline interlock override button, open the foreline valve and watch the foreline pressure gauge until the pressure is below one torr, an audible click should be heard as the foreline interlock is engaged. After the foreline interlock is engaged, release the foreline interlock override

button, and the medium vac pump should stay on.

Note: If the foreline interlock override button is released before the foreline interlock is engaged, the machine will shut off.

6. When the foreline pressure is below 100 mtorr, press the start button on the turbo pump. It will take a few minutes for the turbo pump to reach normal operation.

7. Allow the turbo pump enough time to de-gas (at least 30 minutes). The foreline pressure should settle in below 30 mtorr and the turbo pump should have a load of less then one amp.

At this point the vacuum system will be in the standby configuration, independent of the state of the chamber.

A.3.2 Venting the chamber

1. Important: Ensure that the nitrogen supply to the vent gas inlet on the back of the machine is no more then 5 psi.

2. Put the system into the standby state (hi-vac valve closed, rough valve closed, foreline valve opened, ion gauge off).

3. Important: Open the latch on the chamber door to ensure there is no chance of over pressurization of the chamber.

Note: If the chamber is over pressurized it is a very dangerous state that can result in serious bodily injury or death.

4. Open the vent valve and watch the chamber pressure until it reaches atmosphere and the chamber door opens.

5. Close the vent valve.

A.3.3 Roughing the chamber and placing the system into hi-vac

1. Ensure the vent valve is closed, and close the chamber door.

2. Close the foreline valve, wait for 5 seconds, then open the rough valve. The sound from the medium vac pump will change as the chamber is pumped down.

3. Carefully watch the foreline pressure, it will rise slightly. If the foreline pressure exceeds 200 mtorr, close the rough valve, wait for five seconds, then open the foreline valve to bring the foreline pressure back down. Repeat this process as necessary to rough out the chamber.

Note: Under normal operation, it should not be necessary to cycle between roughing and standby while roughing the chamber. If the foreline pressure climbs at an exceedingly high rate (greater than 10 mtorr per second), notify technical support.

4. Once the chamber pressure is below 80 mtorr, close the rough valve, wait for 5 seconds, then open the foreline valve and allow the foreline pressure to drop below 50 mtorr.

5. With the system in standby, and the chamber pressure below 80 mtorr, press the button to open the hi-vac valve. Carefully watch the foreline pressure and note the maximum value of the spike in foreline pressure. The chamber pressure should quickly drop out of the range of the convection gauge (less then 1 mtorr).

   Note: If the foreline pressure spike exceeds 800 mtorr, the chamber should be roughed to a lower pressure before opening the hi-vac valve. If the pressure exceeds one torr, the system will shut off.

6. Allow at least 3 minutes for the turbo pump to pump down the chamber before turning on the ion gauge.

With the chamber pressure below 10^{-4} torr, the system is in hi-vac.

Note: The system should be able to reach below 10^{-5} torr in under 10 minutes and have a base pressure below 10^{-6} torr. If this is not the case, the chamber may need cleaned, or there may be a small leak.

A.3.4 Shutdown

1. Push the close button on the hi-vac valve control, and listen to ensure that the hi-vac valve closes and is fully seated. The hi-vac valve indicator light should turn off.

2. Close the foreline valve and ensure that all the valves on the front panel are tightly closed.

3. Push the start/stop button on the turbo pump controller.

4. Ensure the ion gauge is off and switch the main power off.

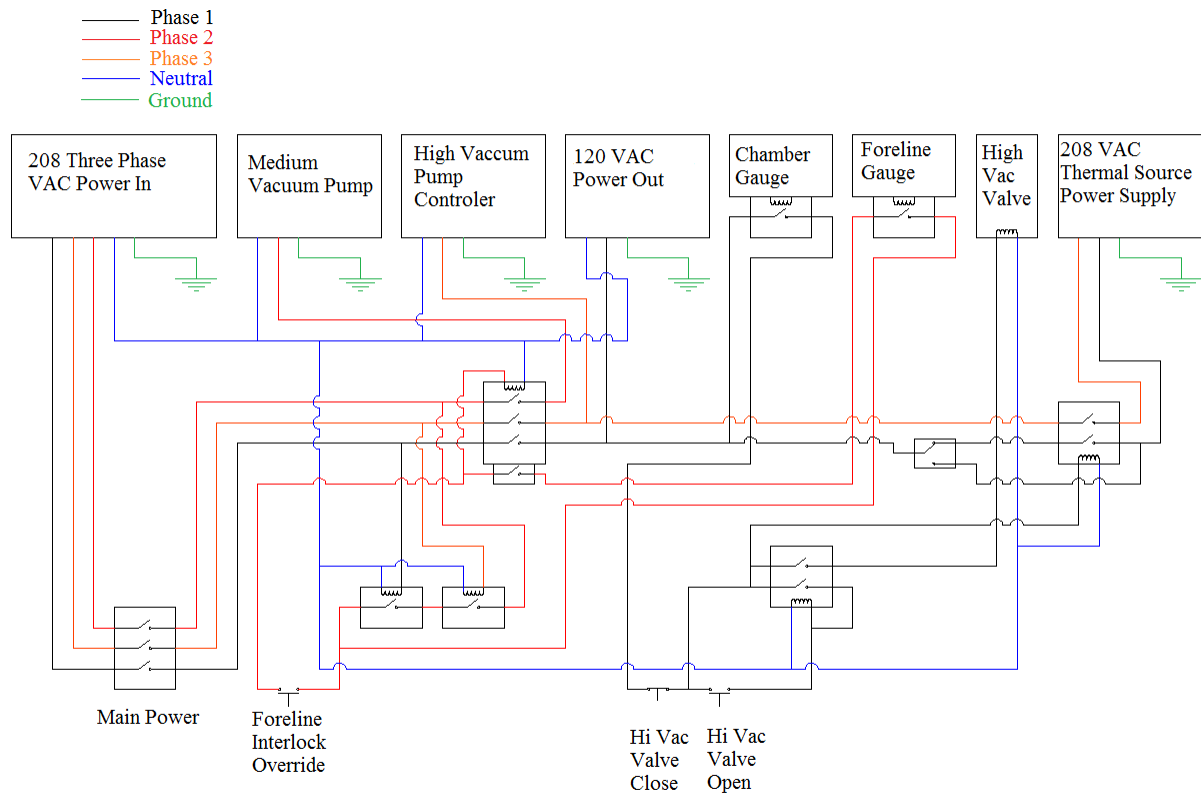## A.4 Interlock Circuit Diagram

Figure A.1: Wiring schematic of the interlock and control circuit

Appendix B

Listings

Simulation/walk3D.py

```
1  """
2  walk3D2.py
3  Created by Casey Hines, May 4, 2013.
4  """
5
6  from simCore import *
7  from mpl_toolkits.mplot3d import Axes3D
8  import matplotlib.pyplot as plt
9
10 def walker(simTime, timestep, walks, speedOfParticle, meanFreePath):
11     """
12     Creates a 3d plot of a set of random walks that are based on the parameters
13     given.
14     """
15     plt.gca(projection='3d')
16     Rsqured = 0
17     expected = 0
18     for n in range(walks):
19         datx = []
20         daty = []
21         datz = []
22         particle = projectile(array([0,0,0]), velocity = speedOfParticle*randomUnitVector(), timestep =
                timestep)
23         t = 0
24         while t < simTime:
25             particle.randomWalk(meanFreePath)
26             if particle.collision == True:
27                 datx.append( particle.position[0] )
28                 daty.append( particle.position[1] )
29                 datz.append( particle.position[2] )
30             t = t + particle.timestep
31         expected = particle.position
32         Rsqured = Rsqured + sum( i**2 for i in particle.position )
33         plt.plot(datx, daty, datz)
34         plt.ylabel('[m]')
35     Ravg = sqrt(Rsqured / float(walks))
36     print Ravg
37
38     #font = {'family' : 'normal',
39             #'weight' : 'bold',
40             #'size'   : 22}
```

```python
41
42    #plt.rc('font', **font)
43    #plt.title('Simulated path of %d particles\n'
44    #'with a mean free path of %s mm \n'
45    #'and average velocity of %s m/s'
46    #%(walks,meanFreePath*1000,speedOfParticle))
47
48    plt.show()
49
50 setSeed(1) # leave blank for random seed
51 # walker(simTime,timestep,walks,speedOfParticle,meanFreePath)
52 walker(1,0.0001,100,100,0.1)
```

<div align="center">Simulation/simCore.py</div>

```python
1  """
2  simCore.py
3  Created by Casey Hines, May 4, 2013.
4  This module provides physical simulation routines.
5  """
6  from pylab import *
7  import time
8
9  class projectile(object):
10    """
11    The projectile class is the general object class for preforming classical
12    simulations. It provides some basic functions for modifying the state of a
13    projectile.
14    """
15    def __init__(self,position,velocity = array([0,0,0]),potential = array([0,0,0]),mass = 1,
            timestep = 1):
16      self.positionPast = position - velocity * timestep - potential * timestep**2
17      self.positionFuture = position + velocity * timestep + potential * timestep**2
18      self.position = position
19      self.velocity = velocity
20      self.speed = sqrt(sum(i**2 for i in self.velocity))
21      self.potential = potential
22      self.timestep = timestep
23      self.mass = mass
24
25    def unconstrainedMotion(self,potential = array([0,0,0])):
26      """
27      The unconstrainedMotion function modifies the position of a projectile based
28      on Newton's laws of motion. The function uses the Verlet integration algorithm.
29      """
30      self.potential = potential
31      self.positionPast = self.position
32      self.position = self.positionFuture
33      self.positionFuture = 2*self.position - self.positionPast + self.potential*self.timestep**2
34      self.velocity = (self.positionFuture - self.positionPast)/(2*self.timestep)
35      self.speed = sqrt(sum(i**2 for i in self.velocity))
36
37    def constrainedMotion(self, positionFuture):
38      """
39      The constrainedMotion function directly modifies the position of a projectile.
40      """
41      self.positionPast = self.position
42      self.position = self.positionFuture
43      self.positionFuture = positionFuture
44      self.velocity = (self.positionFuture - self.positionPast)/(2*self.timestep)
45      self.speed = sqrt(sum(i**2 for i in self.velocity))
46      self.potential = (self.positionFuture + self.positionPast - 2*self.position) / self.timestep
            **2
47
```

```python
48    def randomWalk(self, meanFreePath, potential = array([0,0,0])):
49      """
50      The randomWalk function simulates elastic collisions with unseen particles
51      in which the resulting velocity vector is in a random direction. The probability
52      of a collision is based on the mean free path.
53      """
54      tau = meanFreePath/self.speed
55      # tau is the average time between collisions
56      probabilityCollision = exp(-self.timestep/tau)
57      # the probability of a collision follows a Poisson distribution
58      if rand() < probabilityCollision:
59        self.unconstrainedMotion(potential = potential)
60        self.collision = False
61      else:
62        self.positionPast = self.position
63        self.position = self.positionFuture
64        self.positionFuture = self.position + (self.speed*self.timestep*randomUnitVector())
65        self.collision = True
66
67  def setSeed(*args):
68    """
69    Accepts 0 or 1 argument. 1 argument sets the seed to be used with the random
70    number generator. 0 arguments generated a seed based on the time.
71    Two instances of the random number generator rand with the same seed will
72    produce the same random sequence.
73    """
74    if len(args) == 0 :
75      global seed
76      seed = abs(time.time() - round(time.time()))
77    else:
78      seed = args[0]
79    return seed
80
81  def rand(*args):
82    """
83    Accepts 0, 1, 2 or 3 arguments, returns a quasi random number between
84    0-1, 0-args, or args[0] - args[1]. If three arguments are given, the third is
85    the seed.
86    """
87    try:
88      randomFloat
89    except:
90      global randomFloat
91      if len(args) == 3:
92        setSeed(args[2])
93        randomFloat = seed
94      else:
95        try:
96          randomFloat = seed
97        except:
98          randomFloat = setSeed()
99
100   # Quasi random algorithm
101   x = (pi-3)*2**64
102   M = 2**50 # precision factor
103   randomFloat = ((x * randomFloat + 3.141592653589)%M)/M
104
105   if len(args) == 0 :
106     return randomFloat
107   if len(args) == 1 :
108     return randomFloat * args[0]
109   if len(args) == 2 or len(args) == 3:
110     return randomFloat * (args[1] - args[0]) + args[0]
111
112  def randomUnitVector():
```

```
113    """
114    Returns a unit vector in a random direction.
115    """
116    randomVector = array([rand(-1,1),rand(-1,1),rand(-1,1)])
117    return randomVector/sqrt(sum(i**2 for i in randomVector))
```

Simulation/mfp.py

```
1  """
2  mfp.py
3  Created by Casey Hines, May 4, 2013.
4
5  Calculates and plots the mean free path vs. pressure at a given temperature
6  and collisional cross section.
7  """
8
9  from pylab import *
10
11 T = 298.15                 # [K] Room temperature
12 sigma = 8.0e-20            # [m^2] N2 to N2 collisional cross section
13
14 def mfp(T,P,sigma):
15    kb = 1.3806e-23         # Boltzmann constant [m^2 kg s^-2 K^-1]
16    return kb*T/(sqrt(2.0)*sigma*P)
17
18 P = zeros(1500)            # Initialize the data arrays
19 l = zeros(1500)
20
21 for i in range(0,1500):
22    P[i] = 1e-10 * 10**(0.01*i)   # An array of pressures is created
23    l[i] = mfp(T,P[i],sigma)      # An array of mean free paths are created
24
25 P = P*0.00750              # Convert Pa to Torr
26
27 fig = figure(1, figsize = (10, 6))
28 plot(P,l)
29 xlabel('Pressure [Torr]',fontsize = 20)
30 xscale('log')
31 grid(True, which = 'minor')
32 ylabel('$\lambda$ (mean free path) [m]',fontsize = 20)
33 yscale('log')
34 grid(True)
35 grid(True, which = 'minor')
36 show()
```