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Better Beams Through Simplicity: High-intensity Free-Jet Sources in Neutral Atom Microscopy

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in partial fulfillment of the requirements for the degree of

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Thesis Advisor
Erik Sánchez

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Abstract

A novel design for a high intensity micron-scale supersonic free-jet source is described. This design has been implemented in a scanning helium neutral atom microscope at Portland State University, but has not been otherwise investigated. It is proposed that removing the skimmer component of a free-jet source can, under correct operating conditions, allow a comparable intensity beam to be created at greatly reduced complexity. The dsmcFOAM OpenFOAM solver was used to used to model rarefied gas dynamics of skimmed and un-skimmed helium atom sources. This modeling suggests that gas-gas scattering and shock structures occur in un-skimmed sources but can be compensated for with small aperture diameters and high source flow rates. If the comparable operation of skimmed and un-skimmed sources can be demonstrated it will greatly reduce the cost and complexity of helium atom sources for neutral atom microscopy and other applications.

Thesis Supervisor: Erik Sánchez
Title: Associate Professor

Acknowledgments

I am grateful to Philip Witham who designed and built the first functioning pinhole style neutral atom microscope and suggested this project. Thanks as well go to Professor Erik Sánchez for advising and helpful discussion on modeling techniques. Funding for this work was provide by the National Science Foundation's Research Experiences for Undergraduates Program and the Intel corporation. This work was supported by the National Science Foundation under Grant No. 1004737.

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Chapter 1

Introduction

Observations of nature form the basis of scientific inquiry; improvements in optics and imaging systems enhance the researcher's ability to view natural processes and are thus of fundamental importance to the natural sciences. The shift to using massive particles such as electrons and ions for imaging has given investigators radical new capabilities to the point that obtaining atomic level resolution has almost become routine in the modern materials science laboratory. Imaging using slow moving neutral particles such as helium atoms offers the further advantages of very small kinetic energy, non-interaction with electromagnetic fields, and greatly reduced sample preparation requirements. The difficulty in using neutral atoms for imaging comes from the lack of developed atomic optics technology to focus and manipulate atomic beams. The style of neutral atom microscope (NAM) I discuss in this thesis avoids the problem of atomic optics by using a micron-scale supersonic free-jet expansion of helium atoms which is reduced to a sub-micron beam as it passes through a final aperture. This source is much simpler than the typical high-intensity free-jet source which has an additional skimmer component and has not been investigated experimentally or computationally before this work.

In this thesis I first provide background material on Neutral Atom Microscopy (NAM), rarefied gas dynamics and the Direct Simulation Monte Carlo (DSMC) modeling method. After this I review relevant current literature on NAM and describe how my work build from this. I the next chapter I describe the computational and analytical methods I use to investigate NAM sources. After this I present evidence collected from many gas dynamics simulations performed using DSMC and compare them with current analytical and experimental results. In this work I attempt to determine whether a skimmer-less free-jet source can produce a superior helium atom beam for NAM.

1.1 Neutral Atom Microscopy

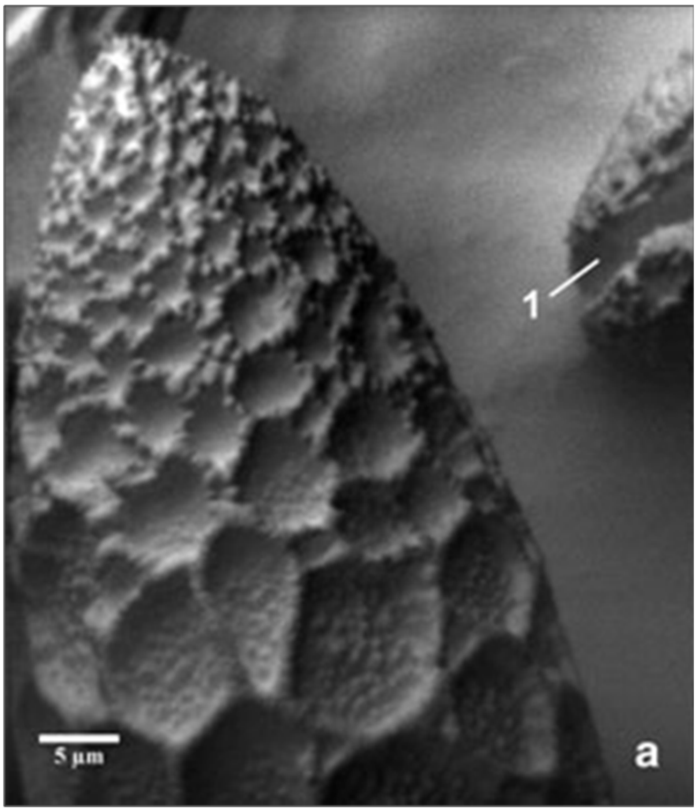

Figure 1-1: A NAM micrograph of a pollen grain. No special sample preparation or coating was used. From: Witham PJ, and EJ Sánchez. 2012. "Increased resolution in neutral atom microscopy". *Journal of Microscopy.* 248 (3): 223-7.

A fundamental constraint on imaging systems is the diffraction limit of the wavelength of particle used to probe the sample [6]. Simply expressed this constraint gives an approximate maximum resolution of half the wavelength of the light used to image. Visible frequencies of light have wavelengths between 400 and 700 nanometers so are fundamentally limited to imaging to hundreds of nanometers in resolution without using special techniques to circumvent this restriction. Imaging with massive particles is diffraction limited by the de Broglie wavelength, being proportional to the inverse

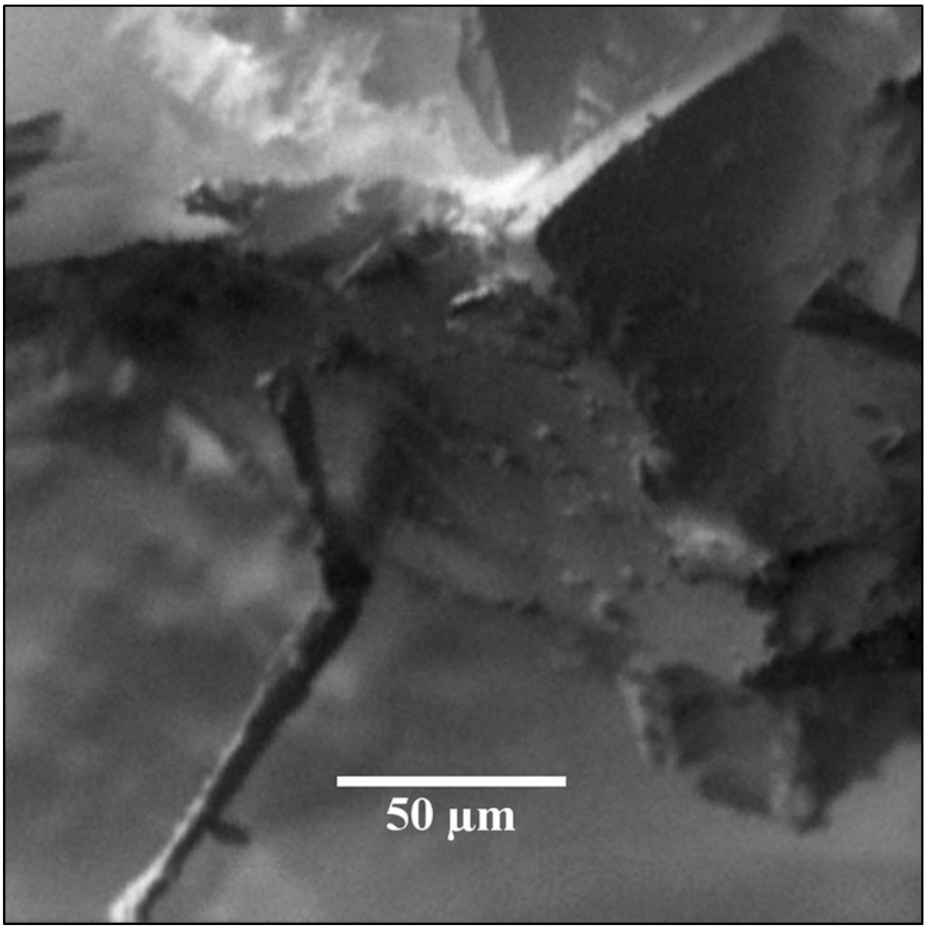

Figure 1-2: A micrograph of a crushed neodymium magnet, neutral helium atoms are unaffected by magnetic fields. Atoms in the NAM beam have less than 0.01 eV of kinetic energy so will not damage samples. From: Witham, Philip, and Erik Sanchez. 2011. “A simple approach to neutral atom microscopy”. *Review of Scientific Instruments.* 82 (10): 103705.

of the momentum, thus requiring either fast moving or heavy particles to reach high resolutions.

For electrons the high velocity of the particles allows the momentum to be large and the maximum resolution very small (well below single nanometer in commercial systems). The mass of a helium atom is around 7000 times larger than an electron, allowing, in principle, the same maximum resolution to be achieved at greatly reduced velocities and thus kinetic energies. The low kinetic energies (less than 0.1 electron-volts at room temperature) of the helium atoms used in NAM allow samples to be imaged without risk of damage or modification. In comparison charged probe particles such as electrons and helium ions have typical energies in the range of thousands to hundreds of thousands of electron-volts. The low energy of the probe particles also allows investigation surface layer properties to delicate to probe using other methods. The NAM is also capable of imaging un-coated samples such as the pollen grain shown in figure 1-1. Using neutral particles the NAM is able to image objects with high electromagnetic fields such as the crushed neodymium magnet in figure 1-2. The major disadvantage of using neutral atoms for imaging rather than ions, electrons or photons is the difficulty in focusing and manipulating the beam. Focusing neutral beams is an active area of research but with one exception [3] has yet to produce micrographs.

In the pinhole style of NAM a high intensity beam of atoms is scattered from a sample and either enters a detector or leaves the sample chamber through vacuum pumps. The signal produced indicates the fraction of atoms scattered into the detector. By scanning the surface of the sample with the beam/detector held fixed, an image can be produced similar to a scanning electron microscope micrograph. Each pixel of the image is produced by holding the beam/detector over a portion of the sample until a sufficient number of atoms have been detected to determine the topology of that portion of the sample. The limiting factors of this design are the intensity and beam diameter of the incident beam, the detector efficiency, and how close to the sample the beam/detector can be placed. The detector used in this type of microscope ionizes the atoms and determines the current flow of ionized atoms [2]. This is the first and only type of NAM to be shown capable of general imaging in the laboratory [9][8].

1.2 Free-jet Helium Atom Sources

The standard method for producing a high intensity atomic beam is to allow a high pressure gas to expand into vacuum. As shown in figure 3 the supersonic expanding gas forms shock systems as it interacts with the background gas in the chamber. A skimmer is placed so that its throat opens before the mach disk. This allows only the atoms from the zone of silence of the free jet expansion to impact the final aperture, pumping away the majority of the skimmer scattered atoms and preventing the formation of shock structures at the final aperture (Fig. 1-3).

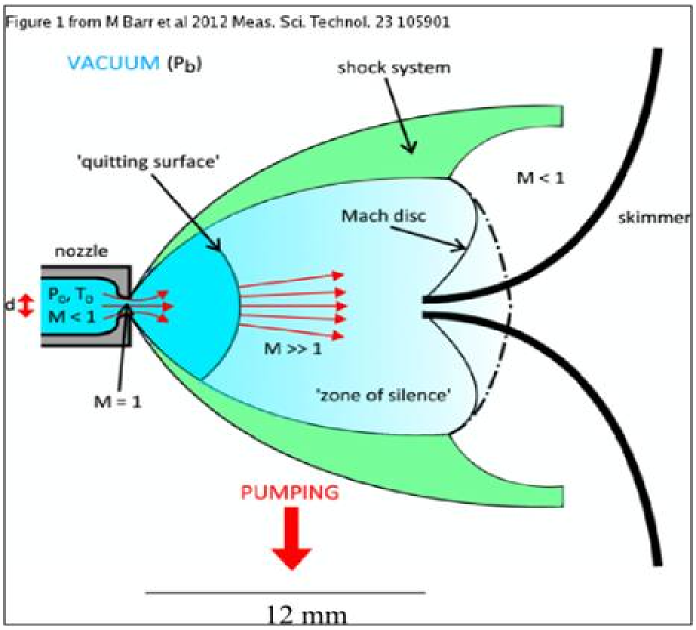

Figure 1-3: A diagram of a free jet helium atom source intended for NAM. The authors used source-skimmer distances of 1.5 to 10 mm and source pressures of 5 to 12 MPa. The nozzle diameter is 2 microns. From: Barr M., Fahy A., Dastoor P.C., O'Donnell K.M., and Allison W. 2012. "A desktop supersonic free-jet beam source for a scanning helium microscope (SHeM)". *Measurement Science and Technology.* 23 (10).

For the creation of Helium beams of interest to building a NAM it was proposed by Philip Witham that with sufficient pumping the free-jet expansion of helium could be keep near the free molecular flow region. This which would allow the skimmer component to be removed from the source with minimal losses due to increased gas-

gas scattering in the source chamber (Fig. 1-4). Removing the skimmer allows the final aperture to be placed much closer to the source nozzle and thus would result in a higher intensity beam. Increasing the beam intensity in a NAM reduces scan time and can allow a smaller diameter final aperture to increase scan resolution.

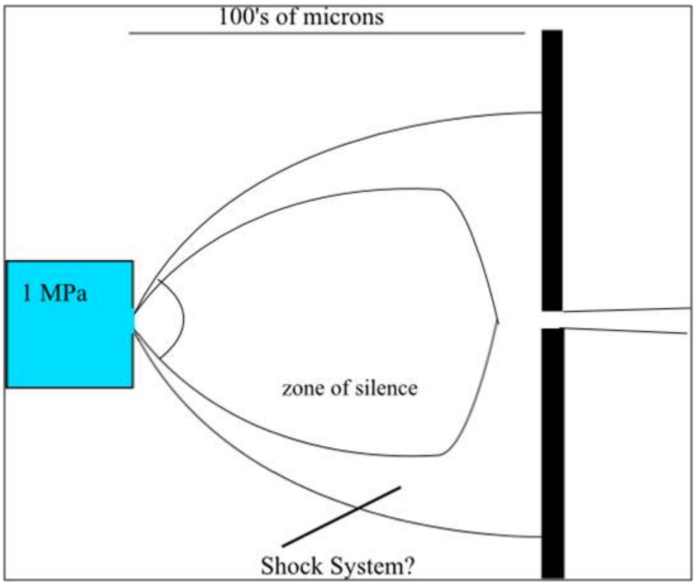

Figure 1-4: Diagram of the type of NAM source currently in use. The skimmer is removed allowing the source to be placed close to the final aperture. The pressure is operated between 1 and 6 MPa and the nozzle diameter is around 0.2 microns

A skimmed free-jet source requires three vacuum chambers and careful alignment of nozzle, skimmer and final aperture. In addition, the distances between the nozzle and final aperture and the placement of the skimmer between these components must be carefully optimized depending on nozzle flow, pumping and chamber geometry[5]. Closed form solutions for ideal arrangements are developed in standard texts on beam source design, but actual sources vary greatly from the theoretical model and are especially difficult to design on the micron scale. In contrast the skimmer-less design has only two vacuum chambers and one distance parameter to be chosen for a given configuration. Alignment of this system is simple to perform as the nozzle can be shifted in space until the maximum beam intensity is reached. This method is also used to find the optimum nozzle-aperture distance for each individual nozzle and gas flow configuration.

1.3 Rarefied Gas Dynamics and Direct Simulation Monte Carlo

Helium gas undergoing free expansion into a low to high vacuum environment is governed by rarefied gas dynamics. The atoms in this expansion have long mean free paths allowing them to travel physically significant distances before scattering from other atoms or surfaces and cannot be approximated using continuum methods.

The dynamics of helium gas in this transition region are difficult to predict with analytical methods and the micron to sub-micron scales of the NAM beam source make precise experimental observations difficult requiring the use computational modeling to compare different beam source designs. The gas dynamics of this region are too complex and the number of atoms much too large to model each atom yet the density of the helium atoms is to low for continuum approximations to be used, the method used in this case is direct simulation Monte Carlo (DSMC). DSMC uses Monte Carlo methods to effectively simulate a small fraction of the atoms in the system and infer gas and molecular properties from this. The DSMC method is well established in aerospace applications for simulations of planes and spacecraft at very high altitudes and is being increasingly used for molecular physics problems [12].

The DSMC method is effective for conditions ranging from highly rarefied free molecular flow to high pressure gases. The degree of rarefication of a gas is described by the Knudson number,

$$Kn = \frac{\lambda}{L}, \tag{1.1}$$

where λ is the mean free path of the gas and L is the characteristic dimension of the system of interest. Knudson numbers greater the than 0.1 indicate that the problem cannot be represented by a continuum model such as Navier-Stokes and require the use of a method such as DSMC [1]. For small Knudson numbers continuum methods are more efficient but DSMC can still be used if the dimensions of simulation mesh can be made small enough to capture the molecular dynamics. DSMC could be used in this way to describe the source nozzle of the NAM where the high pressure helium gas expands into vacuum and transitions to free molecular flow.

A Monte Carlo method, DSMC directly simulates the physics of randomly chosen sample particles to determine macroscopic properties. The primary assumption made by the DSMC method is that particle movement can be decoupled from scattering interactions. In rarefied systems this condition is easily met. The DSMC method is formally described as using Monte Carlo to solve the Boltzman transport equation, but it is implemented and can be understood as directly simulating test particles which capture the microscopic gas behavior. In this processes of alternating steps macroscopic gas properties are used to determine the dynamics of randomly placed test particles which are allowed to evolve for a time step. These particles have dynamics based on the gas being simulated, but corrected for the number of test particles being used to simulate the large number of gas particles. After each time step the results of the dynamical interactions between gas particles are used to determine the macroscopic gas properties of the next time step. This method of simulation provides a full description of gas properties down to the scale of the mesh time and time step used. DSMC can also be modified to account for surface properties of materials and reactions between gas species.

Chapter 2

Method

In this chapter I describe analytical and computational methods I use to investigate the operation of the NAM and compare beam source designs. Closed form solutions exist for ideal skimmed sources, but modeling or experiment must used to investigate non-ideal or novel behavior.

2.1 Analytical results

For ideal free-jet sources closed form solutions of gas properties are available in standard texts[5]. The centerline intensity of a helium atom source of this type is given by

$$I(0) = 3.882 \times 10^{22} \frac{P_0 A}{\sqrt{MT}} \tag{2.1}$$

where P_0 is the stagnation pressure in torr, T is the stagnation temperature in degrees kelvin, M is the molecular weight of helium, and A is the aperture area in cm^2. By driving skimmers with high source pressures high intensity beams can be produced. This intensity is in units of atoms per steradian per second so the particle flux per unit area per second will decrease quadratically as distance from the source increases. A closed form solution for the simple aperture configuration has yet to be developed. If the simple aperture can be described as operating similarly to a skimmed source with some constant attenuation factor then these configurations can be compared. Whether this is a good approximation depends on how the helium atoms in the flow scatter before reaching the aperture. Table 1-1 shows how a simple aperture configuration can outperform a skimmed system even at 1% of the intensity.

Aperture efficiency	Additional length	Skimmer flux	Aperture flux	Ratio
1%	100 μm	5.75×10^{11}	2.075×10^{11}	0.36
5%	100 μm	5.75×10^{11}	1.04×10^{12}	1.8
25%	100 μm	5.75×10^{11}	5.18×10^{12}	9.0
1%	500 μm	3.06×10^{10}	5.75×10^{11}	6.7
5%	500 μm	3.06×10^{10}	1.04×10^{12}	34
25%	500 μm	3.06×10^{10}	5.18×10^{12}	169

Table 2.1: Analytical comparison of 1 μm radius skimmed and simple aperture sources. In the calculations for this table a source pressure of 75000 torr was used with a temperature of 300 K. The flux is calculated on a 1 µm spot at a working distance of 20 µm from the aperture. For skimmed sources the working distance is increased by the length of the skimmer and additional components described by the additional length field. The Ratio field is calculated by dividing the aperture flux by the skimmer flux.

2.2 Modeling with dsmcFOAM

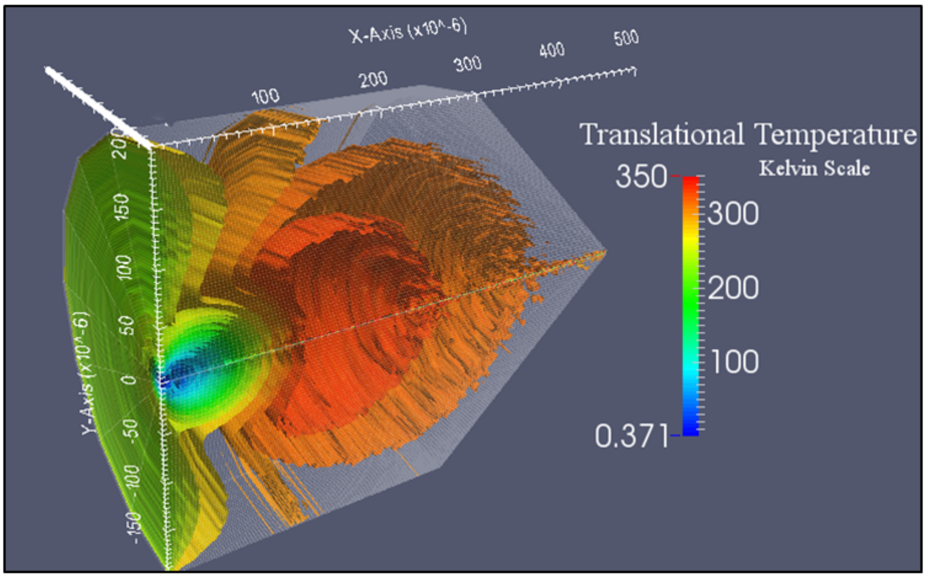

Figure 2-1: An example dsmcFoam simulation of the helium atom beam source in use. This image is taken from the Paraview software and shows the simulation geometry as a transparent wire frame with the temperatures of isothermal surfaces displayed as a heat-map. The front half of the nozzle has been clipped from view. The axis units are microns (also displayed as 10^{-6} meters).

The dsmcFOAM OpenFOAM[13] solver was chosen as a DSMC implementation because it allows full 3-D simulations, runs in parallel using openMPI, and has open source code that can be easily read and modified to fit specific simulation needs. OpenFOAM is a fluid dynamics modeling framework and collection of C++ tools that allow simulations to be designed, conducted and post-processed. This program is open source and designed to be modified to fit the needs of an individual model. In order to perform the simulations for this project I have implemented a modifications to the C++ code in DSMCFoam to better simulate the vacuum conditions needed for this project. I use the DSMCFoam program on the Hydra research cluster based at Portland State University's Academic and Research Computing Department.

The dsmcFOAM program takes exact descriptions of a beam source configuration including geometry, gas sources, and vacuum characteristics and produces a two or three dimensional description of the gas dynamic behavior at each point in simulation time. Simulation geometries can be imported from standard CAD and meshing software such as the Salome platmform[14] or can be hand coded in script configuration files. The simulations conducted use simple geometries, so I chose to use parametric meshes manually refined for each set of simulation parameters. The DSMC method requires sufficient numbers of test particles to be present in each cell, yet becomes inefficient for large numbers of particles in each cell. To meet these constraints the DSMC mesh must be adjusted to have variously sized cells in different parts of the geometry and under different gas conditions. The number of test particles per simulation particle must also be adjusted to insure an accurate simulation that is completed within reasonable time. The dsmcFOAM solver provides a collection of scripts and template simulations that are modified and executed from a command line interface.

The data produced by these simulations are vectors of gas properties at each point in simulation space and time. I selected the Paraview [15] visualization software for post processing of these results. Paraview provides a graphical user interface for interacting and processing simulation results. With this software the full gas properties and DSMC specific parameters of the system including temperature, pressure, gas velocity, number density and many others can be seen at each point in time. This data can be post processed to produce any desirable plots or visualizations needed to understand the system. Figure 2-1 shows an example of the graphics that can be produced from the DSMC results using Paraview. With this software gas properties can be visualized using glyphs such as streamlines or plotted along arbitrary curves.

For this work I perform three-dimensional and two-dimensional simulations using dsmcFOAM. Figure 2-1 is an example of a 3D simulation which attempts to describe the NAM source currently in use at a large scale. These simulations describe the overall gas properties including how pressures and temperatures vary in different regions with changing simulation parameters. The 3D simulations are computationally expensive and complex to process making comparisons between a range of designs difficult. The large scales of these simulations (500 microns in length and 400 in diameter) make precise measurement of beam properties in the 0.1 micron radius final aperture difficult. To investigate the gas dynamics of the final aperture I instead model a similar type of free-jet source using a long thin slit instead of a circular aperture.

Slit gas-dynamics sources can be modeled as a having infinite depth in the long dimension with translational symmetry along that axis. Slit sources allow modeling to be performed in two dimensions with the third accounted for by the geometry of the symmetry. Simulating an infinite slit reduces the number of parameters that can be varied in a simulation and greatly reduces computational difficulty of simulations. Analytical results for infinite slits are well developed [5]. The gas dynamics of a slit source differ from an aperture source primarily in the effect of gas expansion in 2D rather than 3D space. This geometry has a further benefit of making many relations of interest linear rather than quadratic, for example an ideal slit beam loses intensity proportional to distance rather than the distance squared.

To quantitatively describe microscopic rarefied gas dynamics NAM final beam, I make several simplifying assumptions in addition to the infinite slit approximation. In these two dimensional simulations the slit-nozzle is treated as being far away from the final aperture or skimmer so that the incident gas is isotropic along the y-axis and flows at the approximate free expansion limit for helium gas from a free-jet, 1750 m/s. This assumption reduced the number of parameters of the incident gas to one, the number density of the flow. For the simple slit simulations only the slit half-width d is varied and the remaining geometry is held fixed. Similarly for the skimmed simulations only the skimmer half-width is varied.

I use the simple slit modeling results to investigate particular configurations in detail and to compare similar configurations with varying parameters. For individual configurations gas dynamics can be seen in the steady state gas properties such as temperature, density and particle velocity. To compare configurations I take several measurements of the same quantity of each of a set of simulations with a varying parameter and compare them graphically. This can be used to show trends in properties such as final beam intensity as a parameter such as slit width is varied.

Chapter 3

Modeling Results

The dsmcFOAM OpenFOAM solution allows 3D and 2D simulations of rarefied gas dynamics including a full description of gas properties up to the spatial and temporal resolution used. In this chapter I present 3D modeling results of a simulation of the full NAM beam source and 2D modeling results of supersonic gas flows incident on simple slit and skimmer configurations. I examine a special case of each configuration in detail by presenting heatmaps of different gas properties for a configuration and plots of gas properties along and perpendicular to the beam center-line.

3.1 3D results

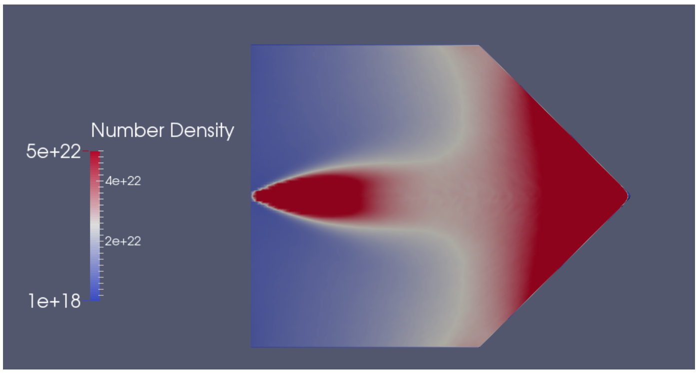

Figure 3-1: A dsmcFoam simulation of the helium atom beam source in use. This image shows nozzle with the front half cut away and helium atom number density shown as a log-scale heatmap. The helium gas is simulated as expanding from a source nozzle at left traveling in along the positive X axis. The source is 500 µm in length and 200 µm in radius.

To qualitatively describe the operation of the helium atom source currently used in NAM I model the entire source from the quitting surface of the free-jet nozzle to the final aperture. These simulations show how the gas density and temperature distributions depend on the combination of large-scale geometry of the beam source and the degree of vacuum pumping and gas flow.

Figure 3-1 shows the NAM source from the quitting surface to the final aperture. In this simulation the nozzle-aperture distance was set to 500 microns. Figure 3-3 shows the translational temperature of the helium atoms during a simulation. This temperature comes from the motion of the atoms relative to the direction of average motion at each position, temperature increases indicate gas-gas scattering and possible shock structures. These source simulations can be used to predict the helium pressure on the final aperture and how much scattering will occur between gas particles before reaching the final aperture.

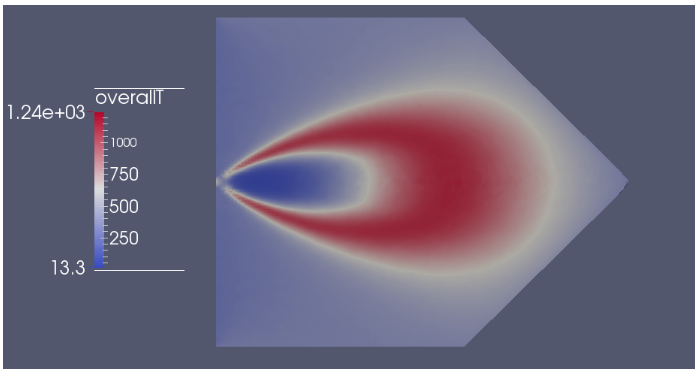

Figure 3-2: This image shows the translational temperature of the helium gas inside the beam source, the gas cools rapidly as it expands into vacuum and then heats from gas-gas and gas-surface scattering. The temperature is measured in degrees Kelvin. This heatmap shows the expected barrel and Mach disk shocks.

3.2 2D results

To investigate the gas dynamics of the final aperture I instead model a similar type of free-jet source using a long thin slit instead of a circular aperture. Slit gas-dynamics sources can be modeled as a having infinite depth in the long dimension with translational symmetry along that axis. Figure 3-3 shows an example of a slit skimmer geometry and figure 3-4 shows an example of modeling results from this geometry The skimmer and final aperture simulations provide a full description of the gas properties during the simulation; to reach steady state gas properties simulations are run until gas properties show only small changes in time. The results in this section are averaged over 0.5 microseconds.

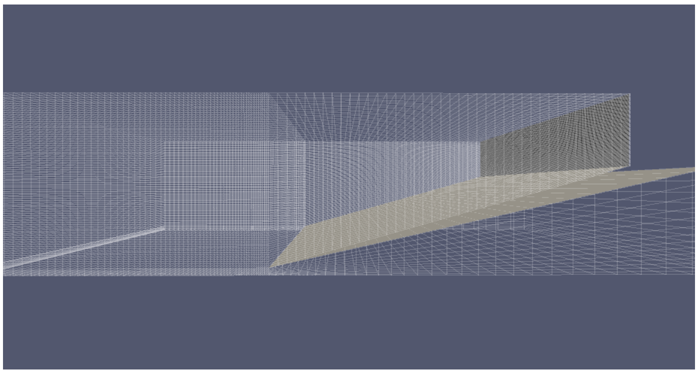

Figure 3-3: An example of a slit geometry with the Z dimension lengthened. In simulations the geometry is symmetric across the y axis so a mirror-symmetry boundary condition can be used at y equal to zero. The geometry is also translationally symmetric along the z axis so the slit can be made thin in the z direction and repeating boundary condition can be used for surfaces facing the positive and negative z directions. The grey surface shows the planes of the skimmer and the wire-frame mesh shows the volume to be simulated.

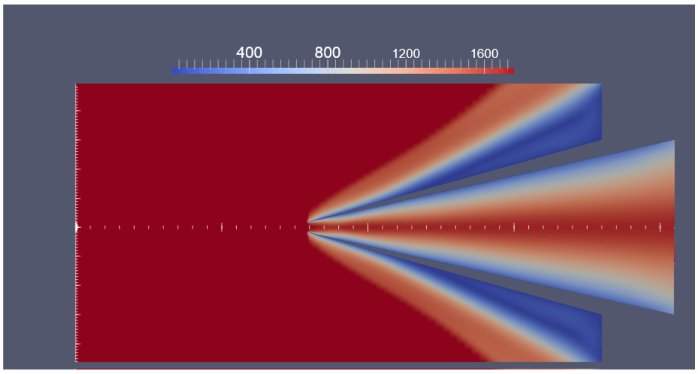

Figure 3-4: A heatmap of the average X direction velocity for helium atoms at each point. This plot shows the simulation reflected across the y axis to show the full skimmer operation. The skimmer in this plot is 100 µm in length, 30 µm in height and has a slit half-width of 2 µm. Helium gas flows from the left isotropically with a number density of 2×10^{25}, an average velocity of 1750 m/s and an initial temperature of 1 K. This simulation has a total length of 220 µm.

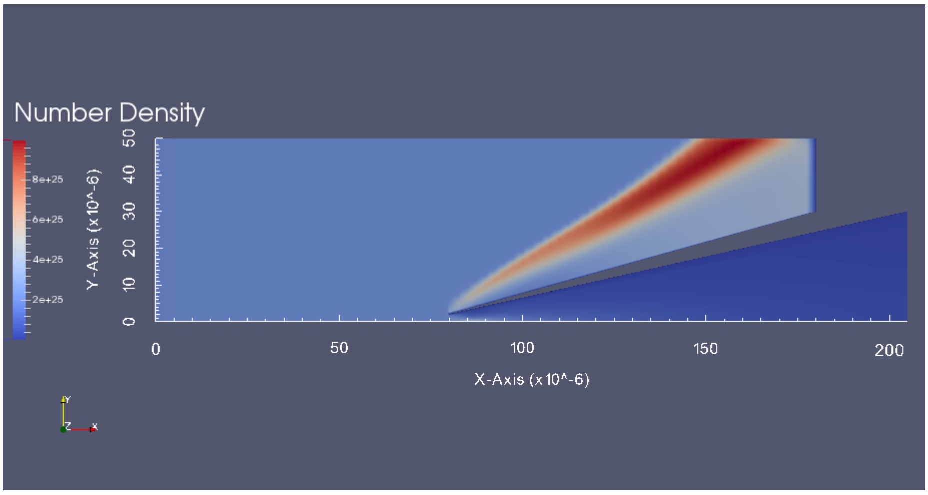

Figure 3-5: A heatmap of the gas number density for helium atoms at each point in a 2 µm half-width slit skimmer. Helium gas flows from the left isotropically with a number density of 2×10^{25}, an average velocity of 1750 m/s and an initial temperature of 1 K.

Figure 3-5 shows the gas number density of a functioning skimmer. Scattered helium atoms are pumped away allowing the skimmer to extract a high quality beam from the zone of silence of the free-jet expansion. The plots in figure 3-6 show average X velocity and translational temperature at each point along the centerline of the same. The skimmer prevents gas scattering from affecting the beam extracted from the flow.

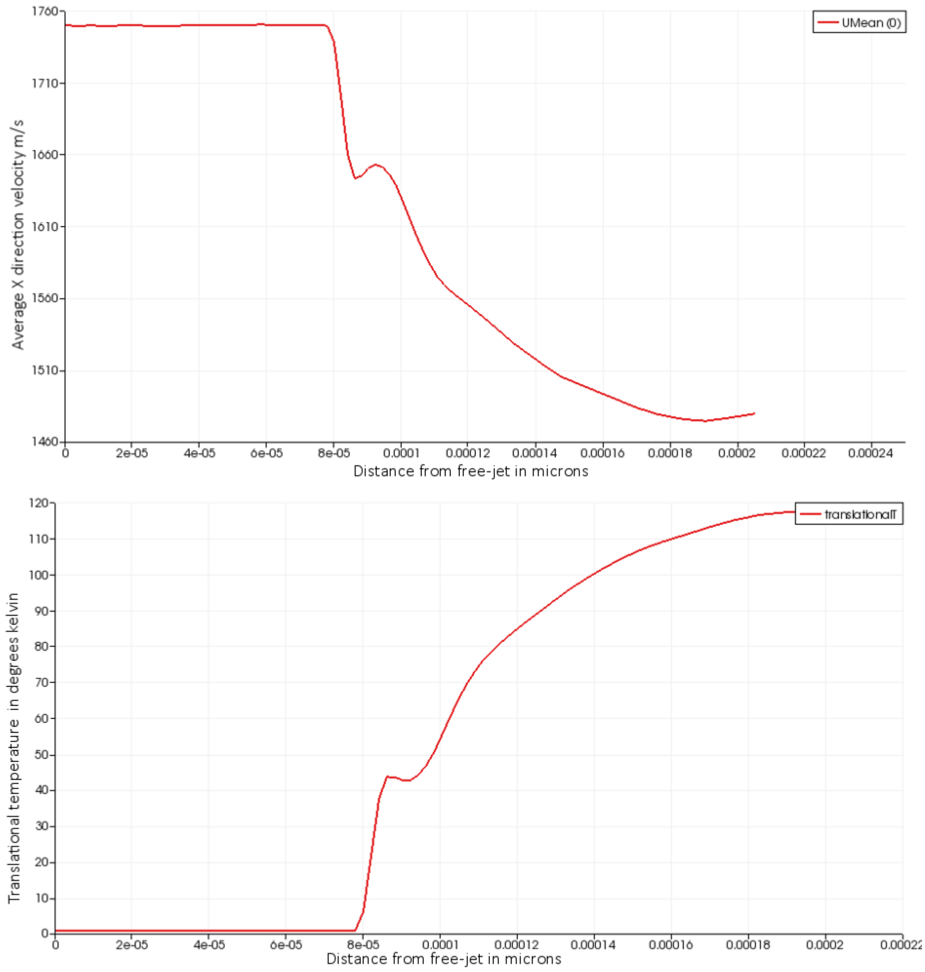

Figure 3-6: Plots of the centerline average X direction velocity and translational temperature of the skimmer shown in figure 3-5. The increase in translational temperature in the throat of this skimmer is caused by operating an an excessive flow pressure for this size skimmer opening. The units in these plots are meters for distance, degrees kelvin for temperature and m/s for velocity.

Figure 3-7 shows a translational temperature heatmap for a simple aperture beam source. To the left of the aperture large number of particles scatter from the incident gas flow and create shock structures and termperature increases, exactly the behavior a skimmer is expected to mitigate. To the right of the aperture the translational temperature in the beam region is very cool. This indicated that the majority of the atoms have passed through the aperture without scattering. This behaivior can also be seen in plots of the temperature and average x direction velocity along the centerline(Fig. 3-8).

Figure 3-7: A heatmap of the translational temperature for helium atoms at each point in a 2 µm half-width simple slit. This plot shows the simulation reflected across the y axis to show the full skimmer operation. Helium gas flows from the left isotropically with a number density of 5×10^{22} , an average velocity of 1750 m/s and an initial temperature of 1 K.

3.3 Comparison simple and skimmed slits in 2D

To investigate how the behavior of a slit configuration is effected by changing a parameter I perform many similar simulations and vary only that quantity. Because of the simplifying assumption used in these models there are only two input parameters for a simple or skimmed slit configuration, the half-width and the flow number density. For simple slits I record the centerline number density and average velocity at at point 20 microns past the slit. For the skimmers I record the same quantities at a point 20 microns past the base of the skimmer which is 120 microns past the skimmer throat. These quantities capture the the intensity and quality (monochromaticity) of the beam. In this section I use these quantities to calculate the beam intensity[1], intensity transmission ratio, and number density transmission ratio. The average velocity is a good direct measure of the quality of the beam, unscattered atoms will have an x direction velocity close to 1750 m/s average velocities less this indicate the presence of scattered particles in a region.

Figure 3-9 shows how the intensity of a skimmed beam varies with the half-width of the skimmer, this linear relation is expected in slit skimmers and is proportional to the area of the skimmer opening in general. Skimmers allow the incident flow to

[1] In this section I use a non-standard definition of intensity as particle flux per square meter, for some applications this is more convenient then particle flux per steradian.

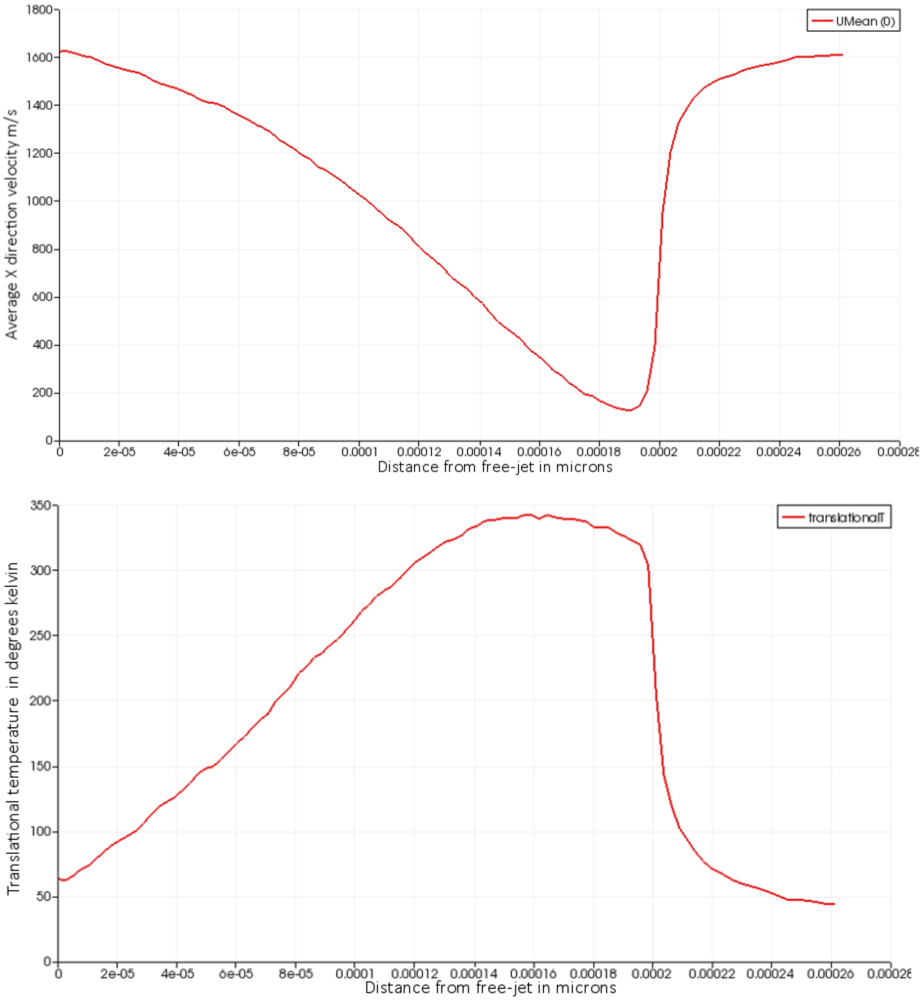

Figure 3-8: Plot of the centerline average X direction velocity and translational temperature of the slit shown in figure 3-6. The large increase in translational temperature along the centerline is avoided in the skimmed design. The units in these plots are meters for distance, degrees kelvin for temperature and m/s for velocity.

Quantity name	Equation	Units
Beam intensity I	$V * N$	$\frac{atoms}{m^2 s}$
Flow intensity I_0	$N_0 V_0$	$\frac{atoms}{m^2 s}$
Intensity ratio	$\frac{I}{I_0}$	Unit-less
Density ratio	$\frac{N}{N_0}$	Unit-less

Table 3.1: Calculated quantities used, N_0 is the flow number density, V_0 is the flow number density, N is the beam number density and V is the beam average velocity.

be increased until the point that gas to surface interactions (not simulated in these models) begin to cause clogging of the aperture. Skimmed source requires that an additional aperture is used to form the final beam for applications such as NAM. For

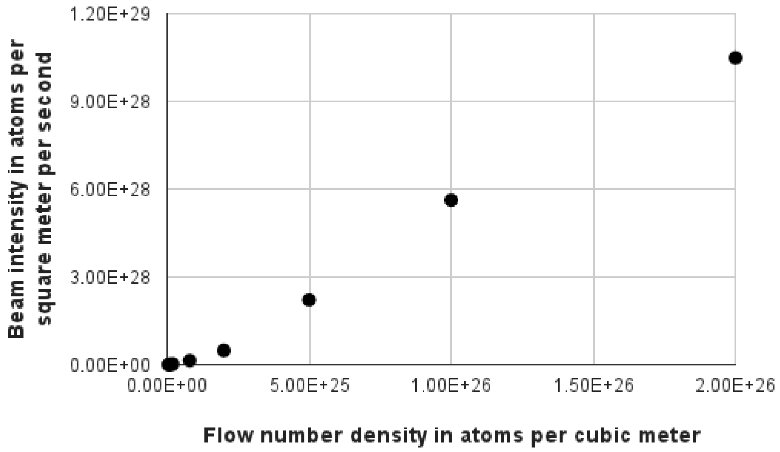

Figure 3-9: A plot of the relation between beam intensity and skimmer opening, this linear relation is expected for a slit skimmer.

high intensity sources a large skimmer opening can be used with a high gas flow and reduced to an effective beam with a small final aperture.

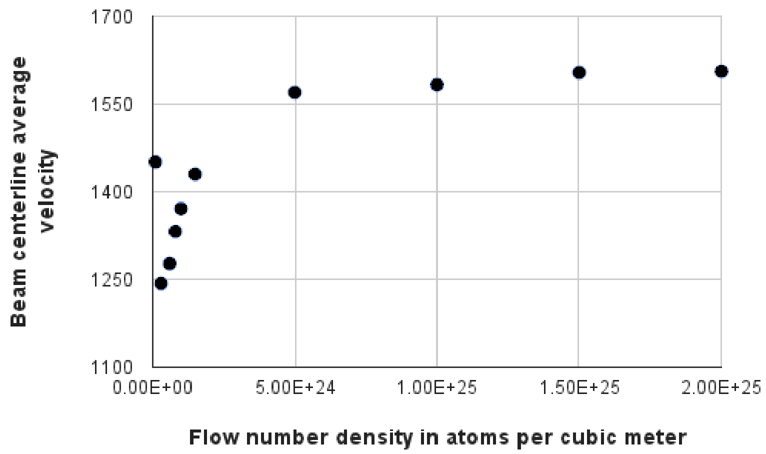

Figure 3-10: Dependence of beam average velocity on flow density for a 3 µm slit. The increase in velocity at high flow rates indicates that the majority of particles in the beam are un-scattered.

As the flow density is increased the average beam velocity at the centerline also increases and reaches a high average velocity (Fig. 3-10). At low flow density the average velocity of the beam increases as the slit is made wider while at higher flow densities the average velocity decreases as the slit is made wider.

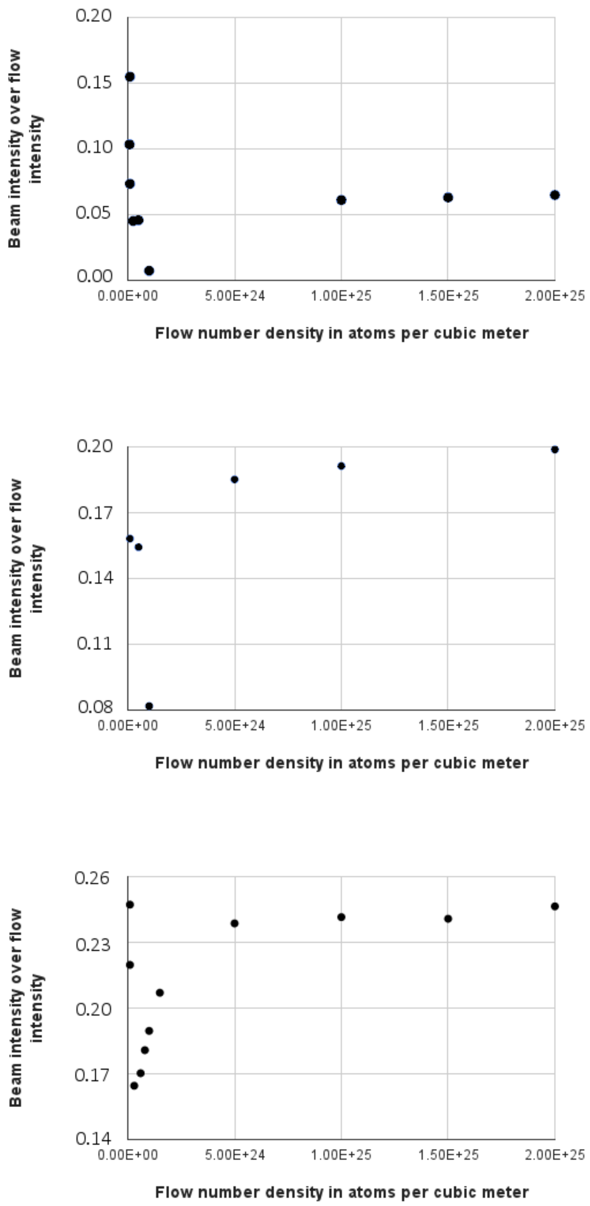

Figure 3-11: Top, intensity ratios for a 1 µm slit half-width. Center, the same for a 2.5 µm slit half-width. Bottom, the same for a 3 µm slit half-width. The increased scattering before the slit results in decreasing intensity ratio with higher flow. For high flow rates the increasing flow results in an increase in the beam intensity ratio.

The plots in figure 3-11 show that the intensity ratio of a simple slit placed in a free jet expansion increases or remains constant as the flow density is increased beyond a critical point. Intensity attenuation does not increase as flow density is increased indicating that the effect of shock structures and gas-gas scattering can be compensated for by operating at high flow rates. The ratio reached at high flow rates varies for different slit half-widths, this is an important quantity that indicates the amount of the incident flow passed through the slit. In figure 3-12 the high flow intensity ratios for different slit half-widths are plotted. The trend line from this plot can be used to estimate the intensity of a given slit and flow rate.

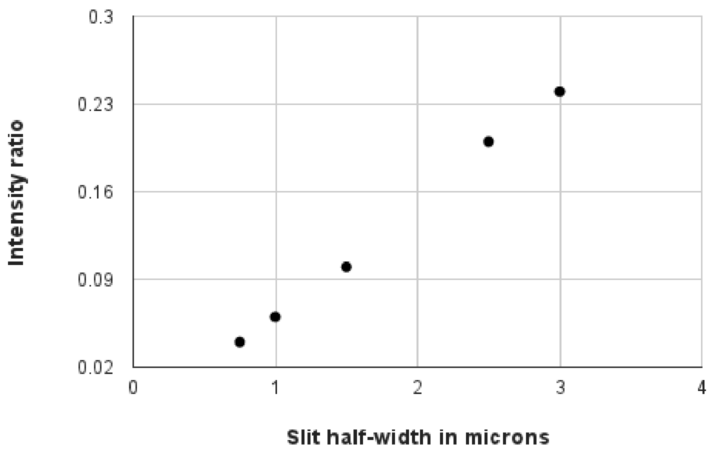

Figure 3-12: A plot of the intensity ratios reached for different slit half-widths.

These results indicate that a skimmer-less free-jet beam source may be able to produce a monochromatic high intensity beam with a much simpler apparatus. In the slit source case the intensity loss due to expansion in free space in one dimension is proportional to the distance traveled, for a NAM beam these losses would be proportional to the distance squared. For some applications such as NAM the attenuation from scattering in front of the simple aperture may be compensated by the reduced geometric losses thus resulting in a higher intensity source.

Chapter 4

Conclusion

In this project I have used the DSMC method to model the properties of NAM beam sources. The results of this modeling suggest that a simple aperture source develops shock structures which increase scattering of the incident gas flow. In the slit case this modeling suggests that beam attenuation from this scattering depends on slit width and flow density. At gas flows beyond a critical point, the amount of attenuation decreases with increasing flow. The beams from these sources were also shown to have a average velocity, similar to the skimmed beams, indicating a high-quality monochromatic beam. From the geometry of gas expanding in three-dimensions I demonstrated that a simple aperture must only have an intensity of several percent of a skimmed source to produce a similar intensity beam. This work suggests that a simple aperture source could produce a molecular beam of comparable or superior intensity to a skimmed source and greatly reduced cost and complexity. High intensity sources are critical to NAM applications and could be used in many other molecular beam physics applications. The current NAM apparatus uses a simple aperture to produce a sub-micron high intensity helium beam but is incapable of precisely measuring beam intensity. By experimentally comparing the relation between gas flow and beam flux for a simple aperture it will be possible to test the results of this thesis. If the ratio of the beam flux over the gas source pressure increases with increasing source pressure it will show that the increased scattering from the skimmer-less design can be overcome and that it is possible to produce better molecular beams from a simple aperture.

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