Loading Buffer-Gas Beams into Traps Using a Single Collision

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1 Introduction

A buffer-gas beam produced from a single-stage cell in the hydrodynamic regime has a large extraction efficiency of $\sim 10\%$ and a modest forward velocity of $v_f \sim 150$ m/s. A small beam divergence is observed for heavy species. The angular spread of the beam scales as $\theta = 2\arctan(\frac{\delta v_t/2}{v_f}) = 2\arctan(\frac{\sqrt{8\ln 2 k_B T/M}}{2v_f})$, where δv_t is the transverse velocity spread of the molecular beam and M is the molecular mass. In addition, using neon as the buffer gas allows efficient cryopumping, leading to a high vacuum in the scientific chamber. With these beam properties, neon-based, hydrodynamic buffer-gas beams have been used in precision measurements.

One possible application of the buffer-gas beams is trap loading. For a molecular beam with mass 20 a.u, a moving velocity of $v_f = 150$ m/s corresponds to a kinetic energy of 27 K. The largest magnetic trap in our lab (the big quadrupole trap) has a trap depth of B_{max}=4 T or 2.7 K for one Bohr magneton species. Apparently, a hydrodynamic beam needs to be slowed down for direct trap loading.

A potential way to load the hydrodynamic beam into the trap without additional slowing is to rely on a single collision happening in the trap center. If the molecular beam collides

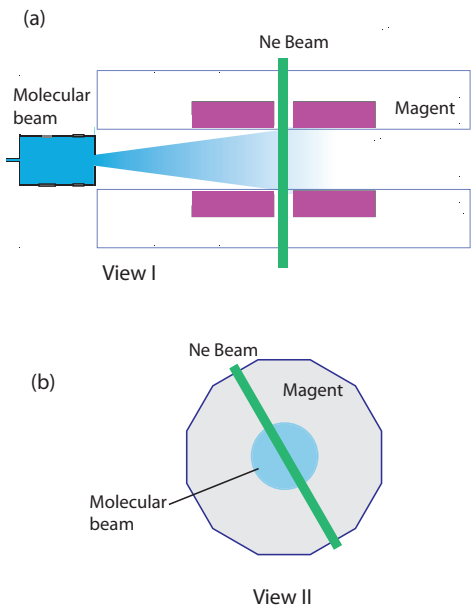

Figure 1: (a) Schematic of loading molecules into a magnetic trap using a single collision between a molecular beam with a neon beam. The molecular beam is sent along the magnet bore and collides with the neon beam which enters the magnet from the midplane. The magnetic trap shown here has a depth of 4 T, with an inner radius of 3.9 cm and a length of 12" (set by the length of its cask). The opening on the side of the magnet for the Ne beam has a diameter of 1 cm. (b) The magnet midplane is shown in cross section. A molecular beam with an angular spread of 30 degrees would fill the magnet bore.

with the other Ne beam, the molecule may end up with an energy lower than the trap depth after the elastic collision. The question is how efficient is the loading process? The first part of this write-up "only" considers the possibilities of creating trappable molecules after the elastic collision. Realistic loading efficiencies using two buffer-gas beams would definitely be lower than the above possibilities due to the molecular divergence and other physical constraints. Fig. 1 shows an experimental setup for loading molecules into a trap relying on cross beam collisions. A hydrodynamic beam has a smaller divergence than a supersonic or effusive beam. However, its finite divergence can still cause collisions to occur outside the trap center, where the local trap depth seen by the molecules after collisions is reduced (or given by $B_{max} - B_{local}$, with collisions happening at B_{local}). Numerical simulations considering the molecular divergence and collisions inside the trap will be shown in the second part of this document.

2 Efficiency of a single elastic collision

Based on the energy and momentum conservation laws for the elastic collision, we can write down the following equations.

$$E_1 + E_2 = E_1' + E_2', \tag{1}$$

$$\vec{p_1} + \vec{p_2} = \vec{p_1}' + \vec{p_2}', \tag{2}$$

where $\vec{p}$ and E ($\vec{p}'$ and E') are the momentum and energy of the particle before (after) the collision. The subscripts indicate which particle is concerned. The momentum conservation relation can be rewritten as

$$\begin{aligned} \vec{p_1}^2 + \vec{p_2}^2 + 2|\vec{p_1}||\vec{p_2}|\cos\theta &= \vec{p_1}'^2 + \vec{p_2}'^2 + 2|\vec{p_1}'||\vec{p_2}'|\cos\theta' \\ \Rightarrow m_1E_1 + m_2E_2 + 2\sqrt{m_1E_1m_2E_2}\cos\theta &= m_1E_1' + m_2E_2' + 2\sqrt{m_1E_1'm_2E_2'}\cos\theta', \end{aligned} \tag{3}$$

where θ (θ') is the angle between the two beams before (after) the collision.

Experimentally, we can measure the initial forward velocities of the cross beams and control the collision angle. This means we can set E_1, E_2, and θ to known values in Eq. 1 and Eq. 3, and only need to solve three unknown parameters, E_1', E_2', and θ' for each experimental condition. There should be various ways to solve this problem numerically. The method I chose is as follows:

(1) For given values of E_1, E_2, and θ, E_1' (molecular's energy after collision) is chosen between 0 and $E_t = E_1 + E_2$.

(2) $E_2' = E_t - E_1'$ is hence constrained by Eq. 1.

(3) Find if a scattering angle θ' exists according to Eq. 3.

(4) Count the total number of scattering events, N_t, and the number of events with E_1' lower than the trap depth, $N_{loadable}$.

Fig. 2 shows the probabilities, $N_{loadable}/N_t$, of molecules with energies lower than the trap depth. Here, three molecular beams colliding with a neon beam (v_f=150 m/s) are calculated. Fig. 2(a) is a special case where where two beams have an identical mass. At a collision angle of 90°, analytical solutions can be obtained. In this special case, Eq. 1 and Eq. 3 become

$$E_1 + E_2 = E_1' + E_2' \tag{4}$$

$$E_1 + E_2 = E_1' + E_2' + 2\sqrt{E_1' E_2'}\cos\theta'. \tag{5}$$

The solutions are

$$E_t = E_1' + E_2' \tag{6}$$

$$\cos\theta' = 0 \rightarrow \theta' = 90°. \tag{7}$$

Molecules with any scattered energy between 0 and E_t can satisfy Eq. 7. The probability of scattered molecules with energy less than the trap depth is hence given by $p = E_{\text{depth}}/E_t$. For two beams moving at 150 m/s and a trap depth of 2.7 K (we assume the magnetic dipole moment is $1\mu_B$ again), $p = 2.7K/(2 \times 27K) = 0.05$, which is consistent the numerical solutions shown in Fig. 2(a).

With this special example, we can also learn that the slower the molecular and Ne beams, the higher the loading efficiency. Of course, a higher trap depth would also increase the efficiency, meaning the single collision loading would be more efficient for more magnetic molecules. Results for colliding CaH and CaF beams with the Ne beam are shown in Fig. 2(b), (c). As the molecular mass increases, the optimal collision angle increases as well.

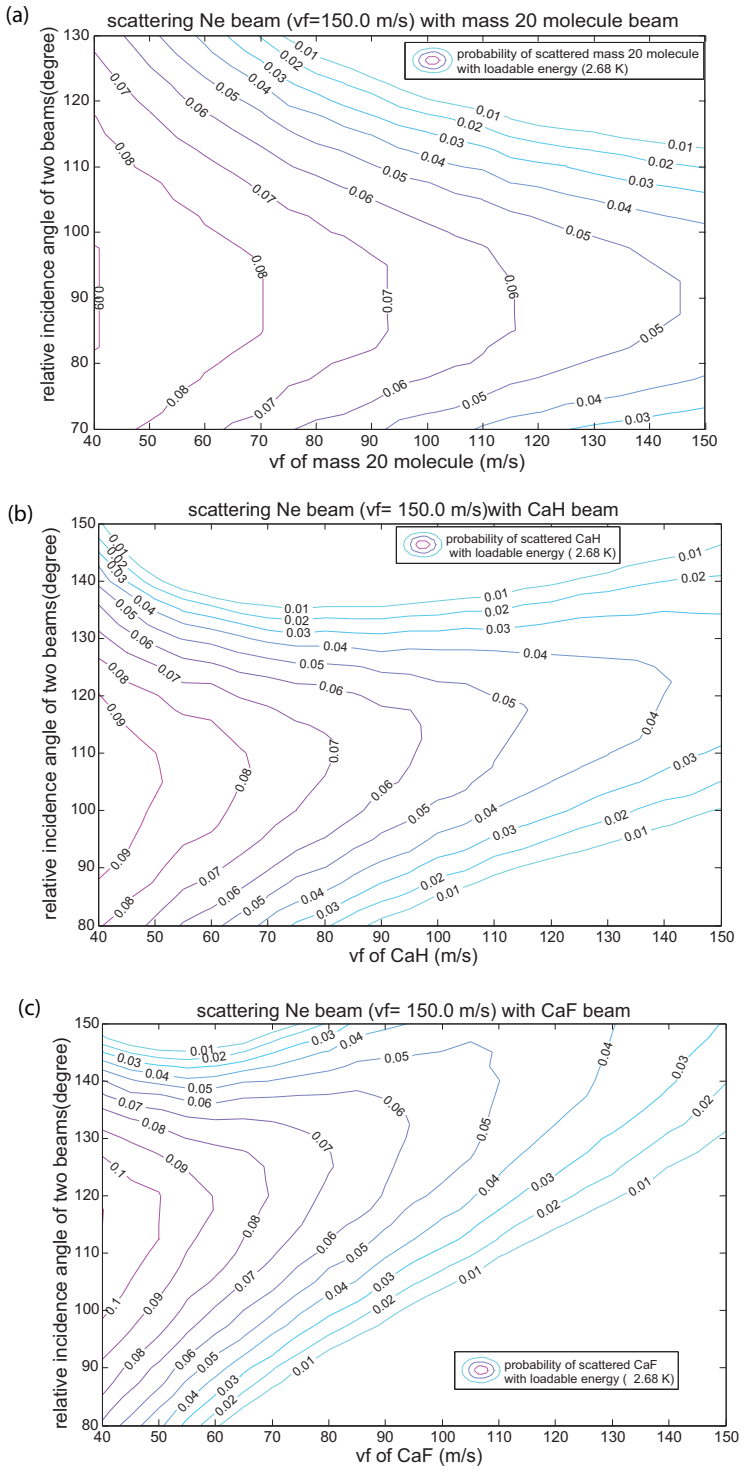

Figure 2: Probabilities of scattered molecules with kinetic energies lower than a trap depth of 2.7 K. (a) Mass 20 molecular beam, (b) CaH beam, and (c) CaF beam collide with a neon beam with v_f=150 m/s. x axis indicates the velocities of the molecules and y axis represents the relative angle of the cross beams, θ.

3 Loading efficiency of the cross Beams

If the molecular beam has a very narrow transverse velocity spread, the probabilities calculated above would be very close to the trap loading efficiency. Assuming the molecular beams are produced from a single-stage cell at a base temperature of 13 K, the corresponding transverse velocity spreads are 120 m/s and 100 m/s for CaH and CaF beams. Assuming the molecular beams has $v_f = 150$ m/s, the angular spreads are 44° for CaH and 37° for CaF. Given the geometry of the big quadrupole trap, a molecular beam placed outside the cask with an angular spread of 30 ° would cover the magnet midplane, as shown in Fig. 1.

Apparently, a full trajectory simulation is needed to know the loading efficiency of molecular beams with finite angular spreads. The trajectory simulation of collision loading is built on top of the simulation codes used for optical loading. First, let's go over some relevant simulation conditions. Fig. 3 shows the orientation of the cross beams and magnet used in the simulations. The magnet is the big quadrupole trap with a depth of 4 T; its bore is aligned along the z axis and centers at $x = 0$. The cell aperture for the molecular beam locates at ($x = X_{\text{cell}}$, $z = 0$) and the molecular beam can be rotated relative to the z axis. Finally, the Ne beam enters the magnet from the side. Since the opening on the side of the magnet has a radius of 0.5 cm and the magnet cask is 3" thick, we can ignore the divergence of the Ne beam and set the radius of the Ne beam to be $r_{\text{Ne}} = 0.5$ cm.

The a trajectory simulation of the loading process contains the following few steps:

(1) Evolve the molecular trajectory starting from the cell aperture until the molecule reaches the Ne beam (or from $z = 0$ to $z = Z_{\text{trap center}} - r_{\text{Ne}}$). This process takes $t = t_1$.

(2) Once the molecule enters the area occupied by the Ne beam ($z > Z_{\text{trap center}} - r_{\text{Ne}}$ and $|y| \leq r_{\text{Ne}}$), we pick a scattering time τ_{scat}, which determines when the scattering event will happen. We check if the chosen τ_{scat} is shorter than the traversing time of the molecule through the Ne beam. If it does, we then move on the next step.

(3) Evolve the molecular trajectory for a duration of τ_{scat}, and then let the elastic collision event occur at time $t = t_1 + \tau_{\text{scat}} \equiv t_2$.

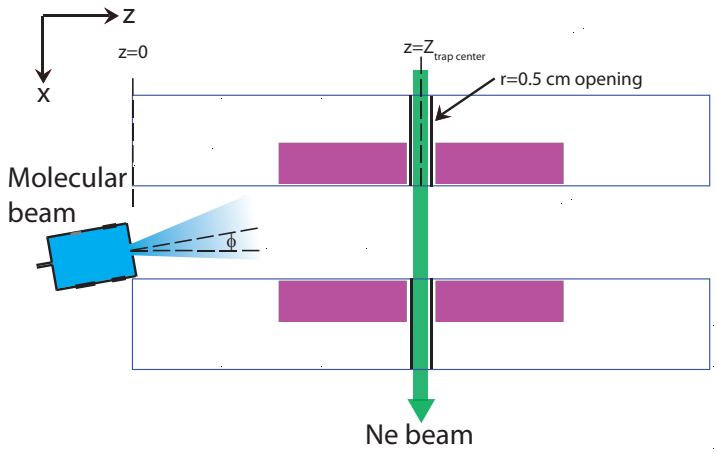

Figure 3: Schematic of the cross beams and the magnet used in the simulation. The magnet bore is along the z axis and centers at $x = 0$. The cell aperture locates at (X_{cell}, $z = 0$) and the trap center is at some distance downstream, $Z_{\text{trap center}}$. The molecular beam axis can be rotated relative to the z axis with an angle ϕ, and X_{cell} can be adjusted. A colliding Ne beam always enters from the midplane of the magnet (its forward velocity is along $+x$ axis).

(4) Keep evolving the molecular trajectory for some time and determine if the molecule stays in the trap.

The codes for the trajectory simulation in the magnetic field are essentially the same for those used in the optical loading simulation. Additional simulation codes are written to treat the elastic collision (Step (2), (3)) inside the trap. (Note: these codes are "CheckScattering.m", "GetScatteringTime.m", and "ScatterParticle.m".) The concepts behind these codes are based on Robert Michniak's thesis.

How to choose the scattering time

When the molecule sees the Ne beam, the mean time between collisions is given by

$$\bar{\tau} = \frac{1}{n_{\text{Ne}} \sigma \bar{V}_{\text{rel}}}, \tag{8}$$

where n_{Ne} is the density of the Ne beam, σ is the molecule-Ne elastic cross section, and $|\vec{V}_{\text{rel}}| = |\vec{v}_{\text{f,Ne}} - \vec{v}_{\text{f,molecule}}|$ is the mean relative velocity. A realistic scattering time would be different from the mean scattering time and can be chosen according to the probability

function

$$P(\tau_{\rm scat}) = \frac{e^{-\tau_{\rm scat}/\bar{\tau}}}{\bar{\tau}}, \tag{9}$$

with $\int_0^\infty P(\tau_{\rm scat}) d\tau_{\rm scat} = 1$.

How to handle the elastic collision

The energy and momentum conservation equations in the center of mass (COM) frame can be written as

$$\begin{aligned} m_1\vec{u_1} + m_2\vec{u_2} &= m_1\vec{u_1}' + m_2\vec{u_2}' = 0 \\ m_1\vec{u_1}^2 + m_2\vec{u_2}^2 &= m_1\vec{u_1}'^2 + m_2\vec{u_2}'^2, \end{aligned} \tag{10}$$

where $\vec{u} = \vec{v} - \vec{V}_{\rm cm}$ ($\vec{u}' = \vec{v}' - \vec{V}_{\rm cm}$) is the velocity of the particle before (after) the collision in the COM frame. The solutions are

$$\begin{aligned} u_1^2 &= u_1'^2 \\ u_2^2 &= u_2'^2. \end{aligned} \tag{11}$$

Eq. 11 tells us that the effect of an elastic collision is to randomize direction of the molecule after scattering in the COM frame. With this concept, we can transform the molecular velocity $\vec{v_1}$ at time t_2 and the velocity of the Ne atom $\vec{v_2}$ (chosen according to the Ne beam properties) to $\vec{u_1}$ and $\vec{u_2}$ in the COM frame. After scattered in the COM frame, the molecular velocity $\vec{u_1}'$ should have the same value before the collision but its direction can be chosen randomly. Finally, we transform $\vec{u_1}'$ back to the lab frame and continue Step (4).

3.1 Simulation results

A special case:

We first use the simulation codes to calculate the loading efficiency of colliding a molecular beam (mass 20 a.u.) with a Ne beam at 90°. Both the molecular and Ne beams have a

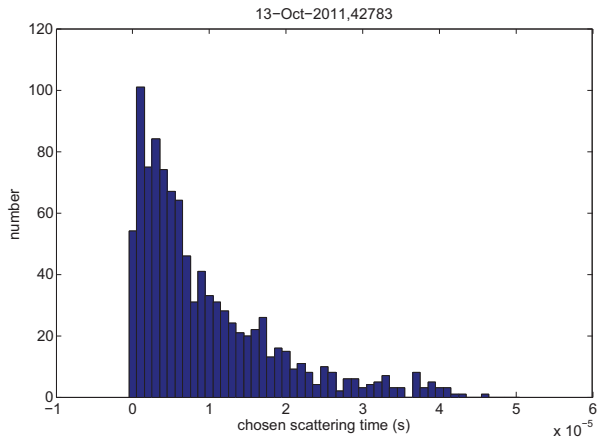

Figure 4: Distribution of the scattering time generated for 1000 molecules colliding with a Ne beam which has a density of $n_{Ne} = 5 \times 10^{14} cm^{-3}$. At this density, the number of scattering time generated is equal to the input molecular number, meaning that a single collision between the molecule and Ne would definitely occur.

forward velocity of $v_f = 150$ m/s; The longitudinal and transverse velocity spreads, δv_l and δv_t, of the molecular beam are set to 2 m/s; $\delta v_{l,\mathrm{Ne}}$ is set to 2 m/s as well. In addition, the distance between the cell aperture to the trap center is $Z_{\text{trap center}} = 15$ cm. In this special case, the beam divergence should have negligible effects and the loading efficiency should be consistent with the results calculated in Section 2. We can also verify if the new codes developed for handling collisions are correct. The distribution of the scattering time generated for 1000 molecules is shown in Fig. 4. The average scattering time for these molecules is 9.36 μs, which is equal to $\bar{\tau}$ in Eq. 8. The loading efficiency for these 1000 molecules is 4.8 %, which is consistent with the results shown in Fig. 2(a). Fig. 5 shows the trajectory of one loaded molecule.

Effect of beam divergence:

Fig. 6 shows the loading efficiency of a molecular beam versus the transverse velocity spread. We can see that the efficiency drops rapidly with increasing beam divergence. Using a 13 K cell to generate a mass 20 a.u. molecular beam would likely produce δv_t=172 m/s. This means the loading efficiency would be even lower than the values indicated in Fig. 6. One way to mitigate the loss due to the beam divergence is to move the cell closer to the trap

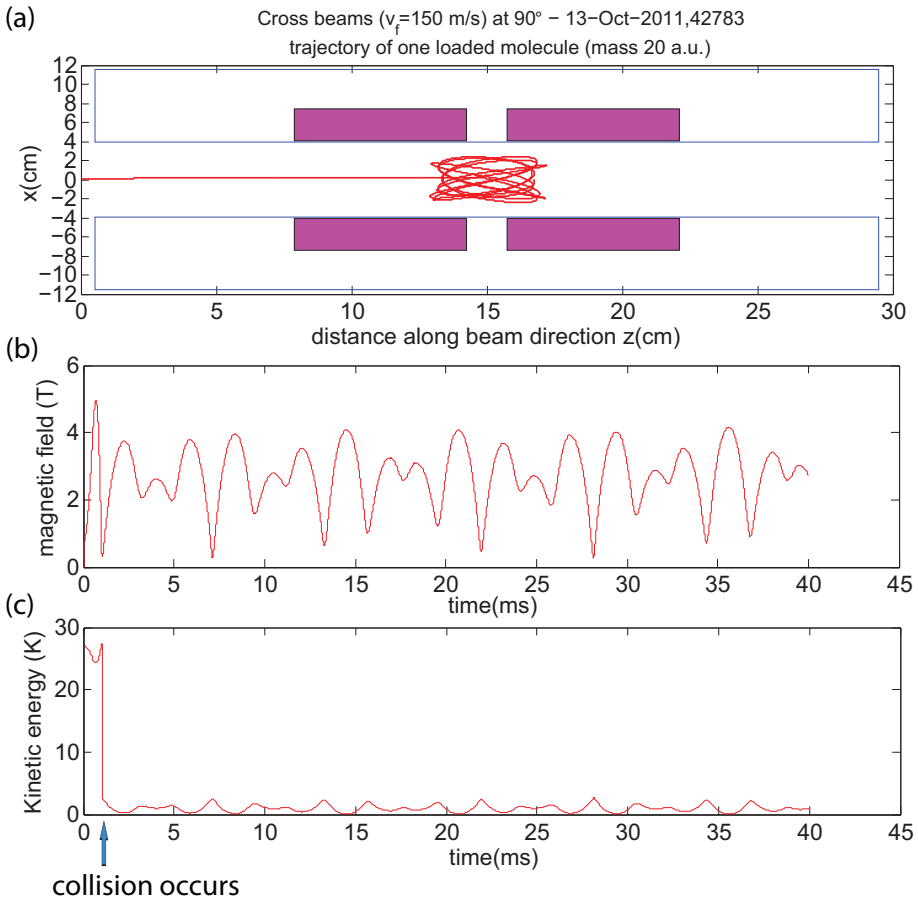

Figure 5: (a) Trajectory of one loaded molecule. (b) Magnetic field experienced by the molecule during the loading process. (c) Kinetic energy of the molecule. Collision occurs at t$\sim$1 ms.

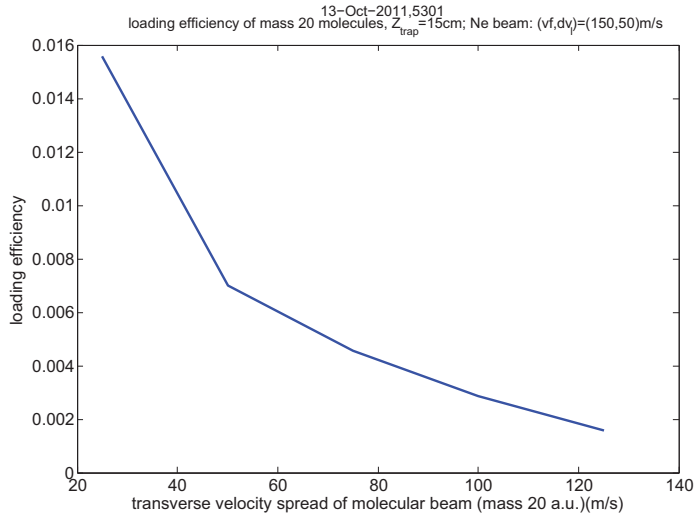

Figure 6: Loading efficiency for a molecular beam (mass 20 a.u.) with increasing transverse velocity spreads. Other molecular beam properties: v_f = 150 m/s, δv_l=50 m/s. Ne beam: v_f = 150 m/s, δv_l=50 m/s, $n_{Ne} = 5 \times 10^{14} cm^{-3}$. Collision angle of the cross beams is 90° and $Z_{\text{trap center}} = 15$ cm.

center. In the real experiment, we could move the cell such that the cell aperture sits outside the saddle of the trap, or $Z_{\text{trap center}} = 5$ cm given by the big quadrupole trap. If we get closer, the loaded molecule would hit the cell in the trap.

Simulation using realistic beams:

Fig. 7 shows the loading efficiency of CaH, CaF, and mass 20 a.u. beams. Here, the trap center locates at $Z_{\text{trap center}} = 5$ cm from the cell aperture. Three molecular beams have a $v_f = 150$ m/s and a longitudinal temperature of 2.3 K and transverse temperature of 13 K. As we learn from Sec. 2, the optimal collision angle would increase for heavier molecules. Therefore, loading efficiency is calculated for different collision angles of the cross beams. The position of the cell along the x axis, X_{cell}, is adjusted as well.

Discussions:

We notice that the loading efficiency for CaH beam is on the order of 10^{-2}. We typically produce 10^{11} CaH molecules in the cell per ablation pulse. Given a 10% extraction efficiency of a single-stage cell, we can load 10^8 CaH molecules per pulse. Loading with multiple pulses is unlikely to be successful since the colliding Ne beam can knock out the previously

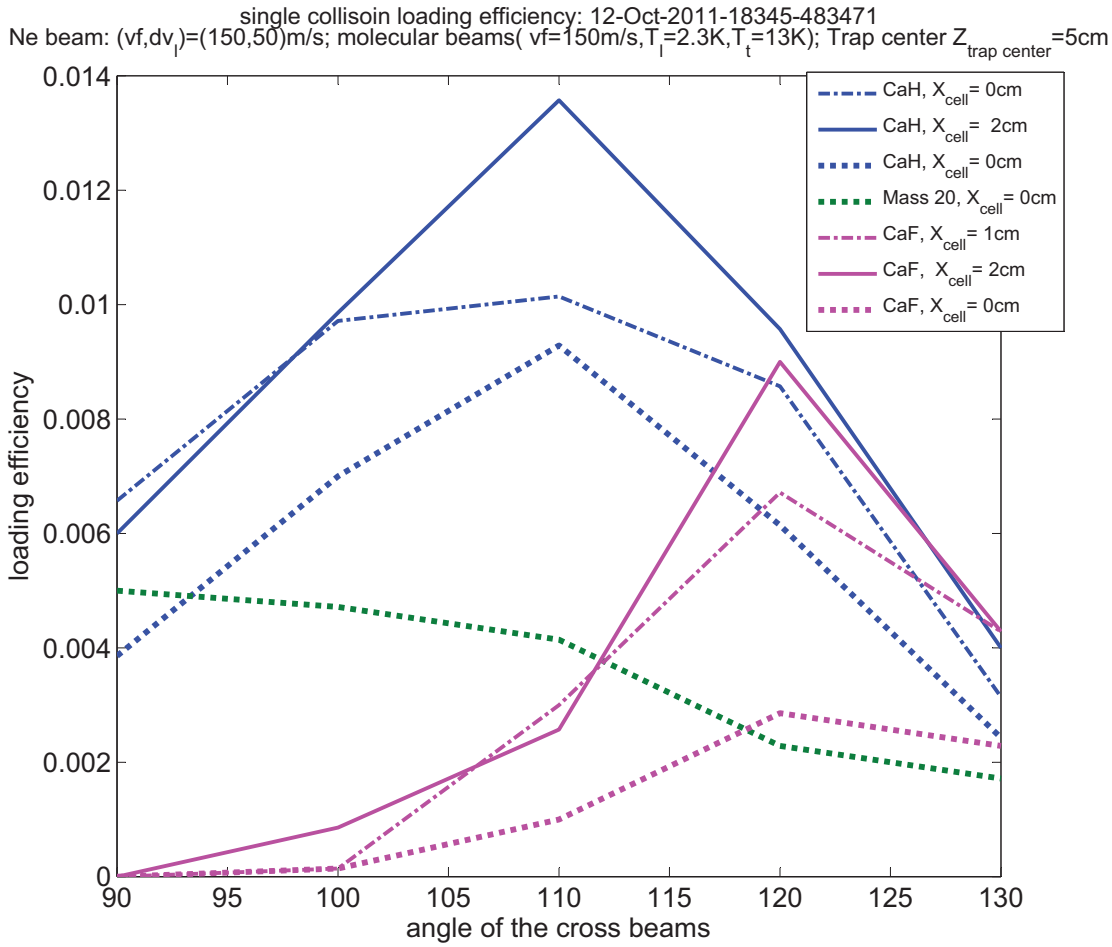

Figure 7: Loading efficiency vs collision angle of the cross beams. Blue, purple, and green curves represent simulation results for CaH, CaF, and mass 20 a.u. beams. The colliding Ne beam properties: $v_f = 150$m/s, δv_l=50 m/s, and $\mathrm{n_{Ne}} = 5 \times 10^{14}\mathrm{cm}^{-3}$.

loaded molecules. However, this method is pretty general since only a single collision is needed. Although the loading efficiency decreases for CaF and mass 20 a.u. molecules, we can always load molecules with better ablation yields than CaH to increase the total loaded number. There is one potential problem with moving the cell to the high magnetic field. At $B = 4$ T, the low-field seeker has a higher Zeeman energy than the high-field seeker by 5.4 K. Although low-field seeking states can be populated in a 13 K cell, there is still plenty of collisions in the molecular beam, which may potentially flip the spin orientation of LFS.