Chapter 4

Isotope selectivity in laser cooling and trapping

4.1 Introduction

For the Alcatraz experiment the isotope selectivity of laser cooling and trapping is of crucial importance. To detect the rare isotope $^{41}\text{Ca}$ at the natural abundance signals from the neighboring $^{40}\text{Ca}$ isotope have to be suppressed by at least 14 orders of magnitude. In this chapter we investigate the isotope selectivity of the various parts of the experiment. In combination these parts have to provide the required selectivity.

Isotope selectivity in laser cooling and trapping is based on the difference in electronic structure between the different isotopes, as was explained in the previous chapter. The momentum transferred to the atom plays an important role and therefore not only the scattering rate but also the detuning of the laser relative to the resonance is important for the selectivity. We will study the isotope selectivity of the compression, the slowing, the deflection and the magneto-optical trapping in this chapter. Numerical simulations have been done to test the selectivity and efficiency of the different parts of the experiment. They will be compared to experimental results in chapter 5.

4.2 Optical selectivity

Optical selectivity for a transition can be defined as the ratio of the fluorescence intensity of isotope 1 at its resonance frequency $\nu_1$ to the fluorescence intensity of isotope 2 at frequency $\nu_1$. As an example the scattering rates of $^{40}\text{Ca}$, $^{41}\text{Ca}$ and $^{42}\text{Ca}$ as a function of the laser detuning are shown in figure 4.1. When the frequency of the laser is tuned to the resonance of one of the hyperfine components of $^{41}\text{Ca}$ also a few $^{40}\text{Ca}$ and $^{42}\text{Ca}$ atoms scatter the light. The difference in the scattering rates determines the selectivity in a single excitation step. The hyperfine structure of the odd isotopes is important because
Figure 4.1: The scattering rates of $^{40}$Ca, $^{41}$Ca and $^{42}$Ca as a function of the laser frequency, assuming equal abundances. For $^{41}$Ca the three hyperfine components ($F=9/2$, $7/2$ and $5/2$) are shown.

the transition strength of the different hyperfine levels is not equal. It was calculated in section 2.2.6 that the ratio of the transition strengths of the $5/2$, $7/2$ and $9/2$ levels is $3:4:5$, and that the transition strength of the $\sigma^+$ transition from the $7/2$ ground state to the $9/2$ excited state of the odd isotopes has the same strength as the $\sigma^+$ transition from the ground state to the excited state of the even isotopes.

The maximum optical selectivity of $^{41}$Ca against $^{40}$Ca reported by Sankari et al [102] for the $^1S_0-^1P_1$ transition is $1.5 \cdot 10^3$. This is clearly not sufficient to allow the detection of $^{41}$Ca at its natural abundance level. There has been considerable interest in the optical selectivity of transitions of the calcium isotopes [102–106] for application in Resonance Ionization Mass spectrometry (RIMS), see also section 1.3.3. In RIMS isotopes are separated using a two- or three-step excitation leading to ionization. The selectivity is further increased by a mass spectrometer. It was shown that an optical selectivity of $2.2 \cdot 10^5$ can be reached using a double-resonance ionization scheme. For an equal excitation rate of two isotopes with an abundance difference of $10^6$ an optical selectivity of $10^6$ in favor of the least abundant isotope is required.

For Atom Trap Trace Analysis the situation is different: here the same transition is excited many times. The total selectivity is therefore greatly enhanced: it is the product of the selectivity of every excitation step. This is the reason that a Magneto-Optical-Trap (MOT), where atoms are trapped by hundreds of thousands of excitation steps, is in principle infinitely isotope selective.

The concept of increased optical selectivity by repeated excitation is illustrated in
4.3 Computer simulations

In order to analyze the isotope selectivity in the various parts of the experiment two computational methods have been used: an average force model and a Monte Carlo model. The most simple approach is the use of the average force on the atoms, as formulated for optical molasses in equation 2.16. Atoms can be traced in small time steps through a light field. After every step the position and velocity of the atom is adjusted. Although this model can give a quick qualitative impression there are important effects which can not be simulated. These effects are the influence of stimulated emission and the heating of the beam due to the discrete nature of the absorption and emission steps. This heating mechanism was discussed in section 2.3.4.

A more advanced model was therefore developed to take into account these effects. In this model we trace the calcium isotopes through laser fields and magnetic fields and calculate at each position the probability of the absorption or emission (spontaneous or

![Figure 4.2: The scattering rates of $^{40}$Ca and $^{41}$Ca compared for 1 excitation step (left) and for 8 excitation steps (right). After 8 excitation steps a distinction can be made by the scattering force between the two neighboring isotopes](image)
Figure 4.3: An example of a part of the trajectory of an atom in the compression stage simulated with the Monte Carlo model. On the top panel the y and z positions are shown, on the lower panel for the same part of the trajectory the velocity in the y-direction is shown. The compression laser is oriented along the y-axis, the atoms mainly have a velocity component in the z-direction stimulated) of photons using a Monte Carlo method. The Zeeman slower, the optical compression and the deflection stage have been simulated using this model. As an illustration of the model we show in figure 4.3 the trajectory of an atom moving through a pair of laser-beams. The atom moves from the left to the right (along the z-axis), while the laser-beams are oriented in the direction of the y-axis. The small jumps that can be seen in the velocity of the atom are due to the absorption and emission of photons.

Features of the Monte Carlo model

In the model the single photon absorption and emission probabilities are calculated. The probability of photon absorption is calculated in each step from the parameters of the light field and the magnetic field at the location of the atom. The position and momentum of the atom are adjusted after the emission and absorption processes. If the atom is in the excited state both spontaneous emission and stimulated emission are taken into account.

The probabilities for emission and absorption are calculated as follows. For a two level atom in a laser field there are three possible processes: absorption of a photon, spontaneous emission of a photon and stimulated emission, where one photon induces the emission of another photon, after which the two travel further in the same direction. For the population of states of the atoms we have

$$\frac{dN_e}{dt} = B_{ge}\nu N_g - AN_e - B_{eg}\nu N_e$$

(4.1)

where $N_e$ is the population of the excited state, $N_g$ the population of the ground state, $A$ the Einstein coefficient for spontaneous emission and $B_{eg} = B_{ge} = B$ is the Einstein coef-
4.3. Computer simulations

As efficient for stimulated emission or absorption respectively, \( u(\nu) \) is the radiation density. \( A \) is equal to \( \gamma \), the spontaneous emission rate, which is \( 2\pi \cdot 34 \text{ MHz} \) for calcium (also \( \gamma = \frac{1}{\tau} \), with \( \tau \) the lifetime of the state), and

\[
B u(\nu) = \frac{s\gamma/2}{1 + (2\delta/\gamma)^2} \tag{4.2}
\]

where \( s = I/I_s \), \( I \) the intensity of the laser beam, \( I_s = \pi\hbar c\gamma/3\lambda^3 \) the saturation intensity (59.9 mW/cm\(^2\) for Calcium) and \( \delta \) the detuning of the laser light with respect to the atomic transition. For one atom the probability of absorption, stimulated emission and spontaneous emission are

\[
P_{\text{abs}} = P_{\text{stim}} = e^{-Bu(\nu)t} \tag{4.3}
\]
\[
P_{\text{spon}} = e^{-At} \tag{4.4}
\]

Limits of the model

The influence of magnetic fields is included, but presently only for the relatively simple case of the even calcium isotopes. The odd calcium isotopes are treated in a simplified way. Only the most relevant hyperfine level is taken into account, and of this hyperfine level only the most relevant sub-state is calculated (which has a simple linear Zeeman shift). Even though we can calculate the splitting and shifting of the three hyperfine excited-state levels for the relevant odd isotopes (\( ^{41}\text{Ca} \) and \( ^{43}\text{Ca} \)) as was shown in figure 2.3, inclusion of these shifts into our model would have taken more time than available at the moment. Why the calculation with this simplification will still give valid results is explained in the following.

When using circularly polarized light to excite the odd Calcium atoms optical pumping will occur. This means that the relative populations of the magnetic sub-states of the hyperfine levels will be modified by the repeated optical excitation and subsequent emission. The reason for this is an optical selection rule: with \( \sigma^+ \) light (right-hand polarized light) only a transition with \( \Delta m_F = +1 \) can be induced. As an example we can look at the excitation of a \( ^{41}\text{Ca} \) atom by \( \sigma^+ \) polarized light, tuned to the \( F = 9/2 \) hyperfine level of the \( ^1\text{S}_0 - ^1\text{P}_1 \) transition. The ground state has \( F = 7/2 \). If we take the initial distribution over the ground state hyperfine sub-levels to be isorotopic, we can calculate the population distribution by multiplying an initial population matrix by the product of excitation and spontaneous emission matrices. The spontaneous emission probabilities have been calculated in section 2.2.6. The relative population in the \( m_F = +7/2 \) hyperfine ground state is found to be 15.6 %, 74.7 %, 97.7 % and 100.0 % for 1, 10, 20 and 100 excitation steps. We can conclude that after 20 excitation steps the only relevant transition for these atoms is from the \( m_F = 7/2 \) to the \( m_F = 9/2 \) sub-state, and that is the transition we take into account.
4.4 Isotope selectivity in compression

The compression of the atomic beam by optical molasses is the first isotope selective stage of the experiment. The purpose of a compression stage is to increase the brightness of the atomic beam by decreasing the transverse velocity of the atoms. To reduce the transverse velocity component of $^{41}\text{Ca}$ atoms we can use laser-beams perpendicular to the atom beam which are about one natural linewidth red-detuned from the resonance frequency of $^{41}\text{Ca}$. This effectively cools the transverse velocity component of the atoms, as explained in section 2.4.1.

When we study the isotope selectivity of the compression we notice that the optical selectivity is not maximized because the laser is not tuned to the maximum scattering rate of $^{41}\text{Ca}$. We expect however a significant isotope selectivity in the optical compression because the laser, when red-detuned for $^{41}\text{Ca}$, is blue detuned for $^{40}\text{Ca}$. The same optical molasses that reduces the transverse velocity of the $^{41}\text{Ca}$ atoms thus increases the transverse velocity component of the $^{40}\text{Ca}$ atoms. And only atoms with a very small transverse velocity can make it to the end of the Zeeman slower and to the trap. For moving atoms we can think of the isotope shift as a velocity shift of the resonance conditions. The isotope shift of 154 MHz between $^{40}\text{Ca}$ and the 7/2 to 9/2 transition in $^{41}\text{Ca}$ corresponds to a velocity difference of 72 m/s.

We have done a simulation of the compression process using the Monte Carlo model in order to find out the optimum parameters for isotope selectivity and efficiency. The schematic layout of the simulation setup is shown in figure 4.4. In the simulation we consider an atomic beam consisting of $^{40}\text{Ca}$ atoms. At a distance $X_1$ from the exit of the oven from which the atoms are evaporated the atoms cross a light field. The light field has a length $X_2 = 1$ cm and the total power in the light field is $P = 5$ mW. Then the atoms drift for a distance $X_3 = 40$ cm to the detection region. The detection region is the trapping region: the area from which atoms are trapped is determined in the experiment by the diameter of the trapping laser beams $X_4$, which is 1 cm. The atoms are randomly started from a position within an area which measures 8 by 8 mm. The initial transverse velocity of the atoms is picked from a random normal distribution with center 0 and a width of 40 m/s.

The maximum transverse velocity that an atom can have and still end up in the detection region depends on the longitudinal velocity. Also the interaction time with the optical molasses depends on the longitudinal velocity. For a typical oven temperature of 650 °C the most probable longitudinal velocity is 600 m/s. This is the initial velocity of the atoms that we used in the simulation. It takes these atoms 1.7 ms to travel from the oven to the detection region. In the same time they are allowed to travel 5 mm off axis: this corresponds to a maximum transverse velocity of 3 m/s. The corresponding maximum transverse velocity for an atom moving at 50 m/s is only 25 cm/s. Important to note is that the velocity associated with the Doppler limit is 42 cm/s. This means that even if the atoms are cooled to the Doppler limit in the optical molasses not all of these slow atoms will make it to the detection region: the efficiency of the transfer is never 100%.
4.4. Isotope selectivity in compression

![Diagram](image)

**Figure 4.4:** A schematic drawing of the setup for the determination of the isotope selectivity of the compression stage

The principle of compression is shown by a few simulation results in figure 4.5. The final position of 10,000 atoms is shown for a number of different laser detunings. The compression laser acts only on the y-position directly. A negative detuning corresponds to a blue detuned laser.

The results of this simulation have been summarized in figure 4.6. In this figure the amount of atoms at a certain y position as a function of laser detuning can be seen. Two line-profiles are plotted at the side of the picture. In the top panel the intensity at the center position (y=0) is plotted as a function of the laser detuning, and in the right panel the distribution of the atoms along the y-axis for a detuning of -15 MHz is shown. At this laser detuning a minimum number of atoms arrives at y=0. The other extreme, maximum compression, is for a laser detuning of about 30 MHz. The area within which there is considerable effect is limited from -50 MHz to +50 MHz, which is smaller than the isotope shift (154 MHz). It is clear that for a given laser frequency we can not have optimal compression of isotope $^{41}$Ca and at the same time maximum defocussing of $^{40}$Ca. The maximum increase of the atom number for a detuning of 30 MHz is a factor of $3.7 \pm 0.2$. The maximum decrease is at least a factor 150, since at the detuning of -15 MHz no atoms are found in the detection region around $y = 0$.

We can conclude from these simulations that the largest isotope selectivity can be obtained for a relatively small blue detuning (10 to 30 MHz) with respect to $^{40}$Ca. The decrease of $^{40}$Ca atoms is a stronger effect than the increase of $^{41}$Ca atoms. The argument for this is that a small velocity change in the compression section is already sufficient to prevent these atoms from reaching the detection region. For the increase of the $^{41}$Ca fraction in the detection region the transverse velocity component of the atoms has to be cooled quickly and completely, which requires more laser power.

Extending the compression to 2 dimensions will increase both the isotope selectivity and the efficiency. The expected total increase in intensity in the detection region for
Figure 4.5: The final positions of a large number of atoms travelling through an optical molasses. Atoms are either pushed to the center of the beam for a positive or red-detuned laser, or pushed to the side by a negative or blue-detuned laser.

two-dimensional compression is a factor of 15. The total isotope selectivity could reach a factor of $15^2 = 22500$. The simulation was done for a distance between compression and detection of 40 cm, in order to compare with experimental results which will be presented in chapter 5. For longer distances the requirements on the final transverse velocity become even more stringent: therefore the efficiency and isotope selectivity gain is expected to increase. The distance from the oven to the deflection stage is roughly 1 meter. The atom flux through the area from which atoms can successfully be deflected to the trap is thus without collimation a factor of $(2.5)^2 = 6.25$ smaller, making the total potential gain a factor of $\sim 100$.

If sufficient laser power were available then the optimum solution would be to have a red-detuned compression stage for efficiency followed by a blue-detuned compression stage for selectivity.

4.5 Isotope selectivity in atomic beam slowing

The purpose of the Zeeman slower is to increase the fraction of atoms that is within the capture range of the MOT. The working principle of the Zeeman slower was explained in section 2.4.3. We have used the Monte Carlo model to simulate the trajectories of the different isotopes through the Zeeman slower to see whether there are any isotope selective effects. The results are shown in figure 4.7. At the final velocity of $^{41}\text{Ca}$ (50 m/s) the intensity of $^{40}\text{Ca}$ is reduced by a factor of $\pm 50$. We therefore conclude that the isotope selectivity of the Zeeman slower is at least a factor of 50. The $^{40}\text{Ca}$ atoms moving slower than 50 m/s have a greatly reduced chance of making it past the deflection to the trap. Most of the $^{42}\text{Ca}$ atoms still move at higher velocities and will not be deflected to the trap as will be shown in the next section.
4.5. Isotope selectivity in atomic beam slowing

Figure 4.6: The distribution of atoms over the y axis as a function of the laser detuning. In this simulation the compressing optical molasses is along the y axis, after which the atoms travel for 40 cm to the detection area.

The different final velocity distributions can be understood from figure 4.8. In this figure the trajectories through the Zeeman slower are given for the three isotopes $^{40}$Ca, $^{41}$Ca and $^{42}$Ca while the laser detuning is optimized for $^{41}$Ca. A number of different starting velocities are shown. For each isotope and velocity there is a point in the Zeeman slower where the Zeeman shift equals the Doppler shift, and the atoms are slowed down from this point on. For the different isotopes with the same starting velocity these points are not the same. For $^{40}$Ca this point is reached first, then for $^{41}$Ca, and then for $^{42}$Ca. At the point where the $^{42}$Ca become resonant with the laser light the magnetic field is steeper than it is at the point where the $^{41}$Ca atoms are resonant, because the slope of the magnetic field increases along the axis of the Zeeman slower, as can be seen from figure 3.12.

For a proper operation of a Zeeman slower care must be taken that the slope of the magnetic field is not too large for the given laser power. If it is too large an atom can not be slowed down quickly enough and it will arrive at a location in the Zeeman slower...
Figure 4.7: The results of a simulation testing the isotope selectivity that can be achieved in the Zeeman slower. The laser detuning is optimized for $^{41}\text{Ca}$. The initial longitudinal velocity distribution is shown in the top panel, the final longitudinal velocity distributions of $^{40}\text{Ca}$, $^{41}\text{Ca}$ and $^{42}\text{Ca}$ are shown in the lower panel.

where the magnetic field strength is not sufficient anymore to cancel its Doppler shift, and thus the atom is lost from the slowing process. To avoid this the minimum possible Zeeman slower length is usually increased with a factor $\mu$, which is on the order of 1.5 to 2.

The minimum length of a Zeeman slower for a given starting velocity is determined by the transition rate, the transition energy and the mass of the atom. It just takes a certain number of absorption-emission cycles to bring an atom to rest. Usually the transition is not saturated because we want to avoid stimulated emission, because in stimulated emission the net momentum transfer is zero. Thus, the minimum length is also determined by the laser power used. This is illustrated in figure 4.9, where the percentage of slowed atoms is shown as a function of the laser power. The data is this figure is the obtained from the computer-simulation of the slowing process inside the Zeeman slower. This simulation was done for different laser powers. An atom is counted as ‘slowed’ if the final velocity is smaller then 75 m/s and not equal to the initial velocity.

It can be seen that below 30 mW the percentage of slowed atoms drops dramatically. This is caused by the above-mentioned effect. The isotope selectivity is expected to be optimal if we operate the Zeeman slower close to this critical value of the laser power.
4.6. Isotope selectivity in atomic beam deflection

The main purpose of the deflection stage is isotope selection. The deflection stage assures that the beam of atoms coming out of the Zeeman slower and the Zeeman slower laser beam are not passing through the MOT chamber. Only the deflected atoms enter the MOT chamber and can be trapped. It is possible to make a selection between the different isotopes in the deflection stage because the Doppler shift is reduced such that the Doppler broadened transitions for the isotopes are smaller than the isotope shift.

The earliest reference to isotope separation by radiation pressure found in the literature is the US-patent of Pressmann [107]. He suggests 'a method of separating of isotopes, one of which selectively absorbs light of a predetermined wavelength comprising directing a beam of light across a gaseous beam comprising a mixture of the isotopes to deflect the selectively absorbing species, and collecting the deflected species'. The first experimental report was published in 1974 [108]. In this paper a dye laser is used to selectively deflect Barium isotopes on the $6s^2 \, ^1S_0 - 6s6p \, ^1P_1$ transition. The efficiency is limited by the rather large transition probability from the $^1P_1$ to the metastable $6s5d \, ^1D_2$ state. The ratio of the rates for the $^1P_1-^1S_0$ and $^1P_1-^1D_2$ transition is just 24. Later some improvements in the excitation scheme were made. Further improvement at that time was limited however due to the unavailability of a suitable laser at the required wavelength [109]. Isotopically selective deflection has also been reported with lithium [110].
Janik et al [111] selectively deflected krypton isotopes from an atomic beam. The maximum enrichment factor they observed in the deflected beam was $1.2 \cdot 10^4$ at a deflection angle of 19 mrad (about 1 degree). The aim of their research was to do photon-burst detection of ambient levels of the rare $^{81}$Kr and $^{85}$Kr isotopes in the deflected beam [112].

The best option for the deflection of a slow calcium beam is a one-dimensional optical molasses [89] inclined by an angle with respect to the atomic beam that damps the velocity components of the atoms in the direction of the lasers. The possibility of large-angle deflection of a calcium beam has been shown by Witte et al. [66]. They deflected an estimated $10^{10}$ atoms/s over an angle of $30^\circ$ with mean longitudinal velocities of 35 m/s and a velocity width of approximately 13 m/s. The transverse velocity of the deflected atoms was close to the one-dimensional Doppler limit. The isotope selectivity of the deflection was not investigated though.

For our experiment we have used the Monte Carlo model to analyze the deflection. As a starting point an atomic beam with an average velocity of 30 m/s has been taken. The atoms are started from a square of 8 by 8 mm in the x-y plane. The initial velocity in the in the x-direction is zero, and the velocity in the y-direction is chosen such that the angle of their total velocity is $30^\circ$ with the y-axis. They interact immediately with a pair of counterpropagating laser beams which cross the atomic beam under an angle of $30^\circ$. The laser has a uniform intensity over its diameter of 1 cm and it has a total power of 5 mW. The laser beam axis is defined as the y axis. The velocity component along the y axis is thus cooled, and the atoms travel 40 cm to the MOT-area along the z axis. Here the position of the atoms is recorded. An example is shown in figure 4.10, where the final position (at $z = 40$ cm) of 1000 atoms is shown. The laser was 40 MHz red detuned with respect to the resonance. Also shown is the initial starting area of the atoms at $z = 0$, the area from which the atoms can be trapped and the minimum expected area.
4.6. Isotope selectivity in atomic beam deflection

Figure 4.10: The final position of 1000 deflected atoms for a laser detuning of 40 MHz. Also shown is the initial starting position of the atoms at a position 40 cm away along the z axis, the area from which the atoms can be trapped and the minimum expected area corresponding to the drift of atoms which are transversely cooled to the Doppler limit.

In this simulation 22% of the atoms ended up in the capture area. For the y-position 97% is within the Doppler limit area, while for the x-position this is only 71%. The reason for this difference is the heating in the x-direction due to the cooling in the y-direction.

The efficiency of the deflection has been analyzed as a function of the laser power, the laser detuning and the initial velocity of the atoms.

The effect of the laser power is shown in figure 4.11. From this figure we can conclude that a laser power of 5 mW is sufficient to deflect the atoms while the spread in the x-position is still modest. For higher powers a considerable larger heating occurs.

The effect of the laser detuning can be seen in figure 4.12. From this figure we conclude that the optimum laser detuning for the deflection is around 40 MHz red detuned, because the deflection in the y axis is still good while the spread in the x-position is already considerably less than for a detuning of 20 MHz. When deflecting $^{41}$Ca with a detuning of +40 MHz the effective frequency for $^{40}$Ca is 40-150=-110 MHz. It can be seen that the average y position for this detuning is roughly 40 cm with a rather large spread. From the limited number of atoms in this simulation (1000) none ended up in the trapping region. Therefore we have done the simulation with larger atom numbers to see what the probability is that a $^{40}$Ca atom will end up in the trapping region with this detuning. Even for 100,000 simulated atoms not a single atom ends up in the detection region. Based on that result we estimate that the isotope selectivity of the deflection stage is at least $10^5$. 
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Figure 4.11: The average final position on the x and y axis as a function of the laser power. Note that the laser power scale is not linear. The spread in the final position is indicated by the distance between the 25% percentile and the 75% percentile, which contains 50% of the atoms.

The effect of the initial velocity is shown in figure 4.13. $^{40}$Ca, $^{41}$Ca and $^{42}$Ca atoms with a range of longitudinal velocities have been traced through the deflection molasses. Plotted in figure 4.13 are the deflection angles as a function of the initial velocity for $^{40}$Ca, $^{41}$Ca, and $^{42}$Ca atoms. In the inset the geometry of the atomic beam and the deflection laser beams is shown. The deflection laser is tuned 40 MHz below the resonance frequency of $^{41}$Ca. While the $^{41}$Ca atoms are deflected well for velocities up to 90 m/s, the $^{40}$Ca are pushed away from the atomic beam axis. This is the main reason that the combination of a Zeeman slower and the large-angle deflection is so effective in selectively deflecting only one desired isotope out of the atom beam. Similar simulations have been done for different laser powers, and it follows that both the isotope selectivity and the efficiency of the deflection stage increase with increasing laser power.

We have to look into the deflection in some more detail in order to explain the behavior of the deflection angle of the $^{40}$Ca atoms. Only the velocity component along the axis of the molasses laser beams (called $v_{mol}$) is affected by the deflection molasses. The $^{40}$Ca atoms are mostly resonant with the molasses laser beam pushing them away from the trap (laser 1, cf. fig 4.13). The number of scattered photons depends on the scattering rate as given in formula 2.14, and on the time the atoms spend in the optical molasses. For the $^{40}$Ca atoms at the given detuning this scattering rate is a Lorentzian with its maximum at $v_{mol} = 50$ m/s. This corresponds to an atom with a longitudinal velocity (called $v_{long}$) of 100 m/s. During the time that the atoms are in the optical molasses $v_{mol}$ will...
change due to the scattering. The atoms can be accelerated to a final $v_{mol}$ which depends on the time spent in the molasses and the linewidth of the transition. The deflection angle is determined by the ratio between $v_{mol}$ and $v_{long}$. The minimum in the deflection angle for $^{40}$Ca atoms around 20 m/s is the region where $v_{mol}$ is limited by the time the atom spent in the molasses. For $v_{long} < 5$ m/s the deflection reaches the maximum possible deflection angle of 60°, i.e. parallel to the molasses laser beams. For $v_{long} > 30$ m/s $v_{mol}$ reaches a maximum value limited by the linewidth of the transition. The deflection angle is then just determined by the ratio of this maximum value of $v_{mol}$ and the initial longitudinal velocity.

### 4.7 Isotope selectivity in a Magneto-Optical Trap

To determine the isotope selectivity in the trap we have to take into account both the actual trapping of the atoms and the way in which they are detected. The trap itself only works for a relatively small detuning of about a natural linewidth to the red side of the transition of the isotope of interest. In this sense the trap is infinitely isotope selective. When we detect the scattered photons from the trapped atoms a small signal from the un-trapped atoms can also be detected. The ratio between the signal of the trapped and the un-trapped atoms is the isotope selectivity of the detection, and it is the limiting factor on the total isotope selectivity of the trap.
Figure 4.13: The deflection angle as function of the initial velocity of the atoms for $^{40}\text{Ca}$, $^{41}\text{Ca}$ and $^{42}\text{Ca}$ atoms

In practice the isotope selectivity of the MOT is thus limited by the ratio of the amount of photons that are scattered and detected from the isotope of interest to the amount of photons scattered and detected from interfering isotopes. In the case of calcium, the amount of photons that can be scattered (and thus collected) from the isotope of interest is limited by the time that it stays in the trap. As explained in section 2.5.2 the amount of scattered photons is, without a repump laser, limited to $\pm 100,000$ photons. How many photons are scattered from a single $^{40}\text{Ca}$ atom arriving at the trap?

From the 100,000 photons scattered by the average $^{41}\text{Ca}$ atom we detect about 180, corresponding to a detection efficiency of $1.8 \cdot 10^{-3}$. This detection efficiency is for the light emitted from the center of the trap; the lens system we use focusses the light from the trapped atoms through a pinhole on the photomultiplier. Light which is not emitted from the center of the trap has a much smaller chance of making it to the detector. The area which is imaged is about 1 mm$^3$. We will assume for simplicity that only light from this volume is detected.

A $^{40}\text{Ca}$ atom moving with a velocity of 30 m/s can spend at most 30 $\mu$s in the trap center. If the effective detuning for this atom is 110 MHz then the scattering rate is about $2 \cdot 10^4$ photons/s (from equation 2.14). This corresponds to an average of 0.6 scattered photons during the time that a $^{40}\text{Ca}$ atom is in the trap center.

When trapping $^{41}\text{Ca}$ atoms the laser is blue detuned for $^{40}\text{Ca}$ atoms, which are therefore actively pushed away from the trap center. It is difficult to estimate the resulting reduction in the amount of $^{40}\text{Ca}$ atoms that arrive in the trap center. It is however safe to assume that the ratio between the amount of $^{40}\text{Ca}$ and the $^{41}\text{Ca}$ atoms that end in the trap center is at least equal to the ratio of the trap area (1 mm$^2$) and the trapping area (1.5 cm$^2$) as defined in figure 4.10. This ratio is 1/150. This number will be higher if $^{40}\text{Ca}$...
4.8. Conclusion

Isotope selectivity

We can now combine the estimated isotope selectivities of the various stages of the experiment. The results of the isotope selectivity simulations are summarized in table 4.1. For each part of the experiment the estimation of the selectivity is shown. The right column is showing the possible isotope selectivity that can be reached if we would have more laserpower available. In that case we could add two compression stages to the experiment, the first compressing the atomic beam at the entrance of the Zeeman slower and the second compressing the atomic beam at the point where it is deflected to the trap. With the present laserpower we can test the compression stages, but we can not run all parts of the experiment simultaneously. The estimates given for the individual parts of the experiment should be seen as an estimate of the order of magnitude of the isotope selectivity, and can be used to compare the different parts of the experiment with each other. Careful simplifications have been made in this chapter to obtain these estimates. Nevertheless these estimates can be used as a valuable guideline for the design and optimization of the experiment.

Efficiency

We can also summarize the information obtained from the simulations on the efficiency of the various parts of the experiment. The efficiency is defined as the ratio of the number of $^{41}$Ca atoms that are detected to the total number of $^{41}$Ca atoms that leave the oven. This number is of importance for the total time that a measurement of $^{41}$Ca at the natural

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**Table 4.1:** The outcome of the simulations of the isotope selectivity. The different components of the experiment are shown. Also indicated is the isotope selectivity that becomes possible by adding two compression stages to the experiment. ‘/’ indicates that this component is not implemented.

<table>
<thead>
<tr>
<th>Part of the experiment</th>
<th>Estimate from simulation</th>
<th>present</th>
<th>possible</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression@oven</td>
<td>/</td>
<td>2 · 10^4</td>
<td></td>
</tr>
<tr>
<td>Zeemanslower</td>
<td>50</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>Deflection</td>
<td>10^5</td>
<td>10^5</td>
<td></td>
</tr>
<tr>
<td>Compression@deflection</td>
<td>/</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Trapping</td>
<td>2.5 · 10^7</td>
<td>2.5 · 10^7</td>
<td></td>
</tr>
<tr>
<td>Total Isotope selectivity:</td>
<td>1.2 · 10^{14}</td>
<td>2.5 · 10^{19}</td>
<td></td>
</tr>
</tbody>
</table>

atoms are actively pushed away from the trap center, and lower if not all $^{41}$Ca atoms are collected in the trap center.

Combining the numbers above we end up at an isotope selectivity of the detection of the isotopes in the trap of at least 25 · 10^6.
abundance level would take. The results are shown in table 4.2, where again in the right column the values are shown that can be obtained if we would have enough laserpower to add the two compression stages to the experiment.

For the first step from the oven to the Zeeman slower the atoms are required to have a transverse velocity smaller than 5 m/s. With this transverse velocity, and an average velocity of 300 m/s these atoms can still make it to the exit of the Zeeman slower. The fraction of atoms in this transverse velocity range is estimated at $4 \cdot 10^{-3}$, where we approximate the transverse velocity distribution by a normal distribution with $\sigma = 60$ m/s. This number is based in the compression ratio of 1/10 by the exit channels of the oven.

The 2D-compression stage can increase this fraction by an expected factor of at least 100, depending on the laser power available. However, due to the slowing process in the Zeeman slower we lose some of the atoms: the atomic beam spreads in the transverse direction. Even though the transverse velocity is not so much affected we see a reduction by at least a factor of 10 if we compare the number of atoms at the beginning and the end of the Zeeman slower within a radius of 0.5 cm around the central axis. This simulation result is shown in figure 4.14. Furthermore, the fraction of atoms slowed down to the design velocity depends strongly on the available laser power.

The deflection transfers at most 22% of the atoms from within an area of 8 by 8 mm to the trapping area. In this simulation the longitudinal velocity is 30 m/s and the initial transverse velocity was neglected. Atoms faster than 90 m/s are not deflected anymore. If at the deflection stage there is any transverse velocity in the x-direction this can result in a large loss. Even if the transverse velocity is fully Doppler limited only 1/3rd of the atoms arrives in the trapping area. Of a beam with a normal transverse velocity distribution with
4.8. Conclusion

<table>
<thead>
<tr>
<th>Part of the experiment</th>
<th>Estimate from simulation</th>
<th>present</th>
<th>possible</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression@oven</td>
<td>0.004</td>
<td>0.4</td>
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<tr>
<td>Zeemanslower - spreading</td>
<td>0.1</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Zeemanslower - slowed fraction</td>
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<td>0.9</td>
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<tr>
<td>Deflection</td>
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<td>0.4</td>
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</tr>
<tr>
<td>Compression@deflection</td>
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<td>1</td>
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<tr>
<td>Trapping</td>
<td>0.2</td>
<td>0.2</td>
<td></td>
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<tr>
<td><strong>Total Efficiency:</strong></td>
<td></td>
<td>$1 \cdot 10^{-6}$</td>
<td>$3 \cdot 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 4.2: The estimated efficiency based on the simulation of the different components of the experiment

A $\sigma$ of 5 m/s as was assumed in the initial part of this efficiency estimation, only 7% have a velocity at or below the Doppler limit.

If the atoms arrive at the trapping area we estimate the trapping efficiency at 20%; the detection efficiency is the last step, and based on the results which will be presented in the next chapter we expect that no atoms are lost at this point anymore.

Depending on the total laser power available the efficiency for a number of scenario’s can be estimated. With enough power available to do 2D compression before the Zeeman slower and at the deflection we expect an efficiency of $3 \cdot 10^{-3}$. It is clear from these numbers how much depends on the compression of the atomic beam, because without this the efficiency drops by a factor 2100 resulting in an estimated efficiency of $1 \cdot 10^{-6}$. 