Theoretical study on isotope separation of an ytterbium atomic beam by laser deflection*

Zhou Min(周 敏) and Xu Xin-Ye(徐信业)†

State Key Laboratory of Precision Spectroscopy and Department of Physics, East China Normal University, Shanghai 200062, *China*

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Isotope separation by laser deflecting an atomic beam is analyzed theoretically. Interacting with a tilted one-dimensional optical molasses, an ytterbium atomic beam is split into multi-beams with different isotopes like ^{172}Yb, ^{173}Yb, and ^{174}Yb. By using the numerical calculation, the dependences of the splitting angle on the molasses laser intensity and detuning are studied, and the optimal parameters for the isotope separation are also investigated. Furthermore, the isotope separation efficiency and purity are estimated. Finally a new scheme for the efficient isotope separation is proposed. These findings will give a guideline for simply obtaining pure isotopes of various elements.

Keywords: isotope separation, ytterbium, optical molasses, laser cooling

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1. Introduction

Rare isotopes are widely used in several fields, such as biomedical research,[1] high-resolution spectroscopy,[2,3] and atomic clocks.[4,5] In recent years, a few methods for isotope separation have been proposed. Pure isotopes can be obtained by accelerator mass spectrometry (AMS)[6] or laser ionization.[7,8] Combing techniques from magnetic spectrometry and nuclear physics, the AMS has an extremely high sensitivity in detecting rare isotopes, however it is very inefficient and space consuming. Although the laser ionization approach also has a high isotopic selectivity, it requires multiple high-power pulse lasers for efficient ionization.

The most efficient method may be the one with a magneto-optical trap (MOT), by using that method, a single isotopic component has indeed been cooled and trapped.[9] Nowadays, isotopes of ytterbium (Yb) can be individually trapped in an MOT to be employed for many precision-spectroscopy experiments[10,11] such as the optical frequency standards.[12] The frequencies of the primary transitions of Yb isotopes have been measured accurately, helping to finely tune the atomic wave functions for various advanced researches.[13,14] The MOT is equipped with a quadrupole magnetic field, and this magnetic field should be switched off during precision measurements, so the observation time is limited due to atoms falling down by gravity.[15] Obviously, a continuous atomic beam will give a longer observation time. Therefore, the isotope separation by using laser deflection of an atomic beam has some advantages, which have been experimentally demonstrated.[16–20] Unfortunately, the detailed theoretical analysis of this kind of isotope separation has not been reported yet.

In this paper, we discuss the possibility of separating the Yb isotopes by using a one-dimensional optical molasses (1D-OM). Interacting with a tilted 1D-OM, an ytterbium atomic beam could be split into multi-beams with different isotopes like ^{172}Yb, ^{173}Yb, and ^{174}Yb. By using the numerical calculation, the dependences of the splitting angle on the molasses laser intensity and detuning are studied, and the optimal parameters for the isotope separation are also investigated. The isotope separation efficiency and purity are both estimated. Finally, a new scheme for the efficient isotope separation is proposed.

2. Ytterbium atomic beam generation

Figure 1(a) shows the schematic diagram of the Yb atomic beam generation. A mount of Yb metal is placed inside an enclosed oven with a small nozzle (diameter Φ_1). A thermal Yb beam is generated through the oven nozzle when the oven is heated to a high temperature. A small mechanical hole with a diameter of Φ_2 is located downstream at a distance of L_1 away from the oven, which works as a collimator controlling the atomic beam divergence.

The atomic beam effusing from the oven nozzle has a modified Maxwell–Boltzmann velocity distribution $f(v) = 2(m/2k_BT)^2v^3\exp(-mv^2/2k_BT)$, where v is the atomic velocity along the longitudinal direction, k_B is the Boltzmann constant, T is the absolute temperature of the heated oven, and m is the atomic mass. The mean velocity is $\bar{v} = (9\pi k_BT/8m)^{1/2}$ with this distribution.[21] By assuming that Φ_1 and Φ_2 are very small, the atomic beam divergence half angle is given by $\theta_d = (\Phi_1 + \Phi_2)/2L_1$ and the mean atomic transverse velocity is $v_\perp = \bar{v}(\Phi_1 + \Phi_2)/2L_1$. The characteristic parameters

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†Corresponding author. E-mail: xyxu@phy.ecnu.edu.cn

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of the oven should be chosen so that the transverse velocity and the divergence can be small enough. They are given as follows: $\Phi_1 = 3$ mm, $\Phi_2 = 6$ mm, and $L_1 = 12$ cm. The beam divergence half angle is $\theta \approx 37$ mrad. At the distance of $L_2 = 8$ cm, the atomic beam will expand to have a diameter of $\Phi_3 = 12$ mm. Then the atom beam interacts with the 1D-OM.

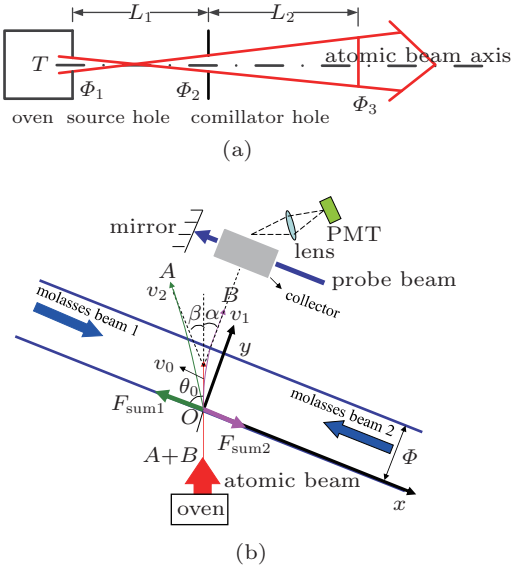


Fig. 1. (color online) Schematic illustration of isotope separation by using a laser to deflect the thermal ytterbium atomic beam. (a) A thermal ytterbium atomic beam effuses from the oven hole of diameter Φ_1 and is collimated by a mechanical hole of diameter Φ_2 at a distance of L_1 away from the oven. The atomic beam is expanded to have a diameter of Φ_3 after a flight of length L_2, where it interacts with the 1D-OM. (b) An atomic beam containing a mixture of isotopes A and B effuses from a heated oven. After travelling through the 1D-OM, the isotopes A and B are deflected from their original trajectories, respectively. The fluorescence signal of the deflected atomic beam induced by a probe laser is detected by a photo-multiplier tube through a lens. Here the probe laser is retroreflected by a mirror.

3. Principle of isotope separation

An atomic beam containing a mixture of isotopes A and B effuses from a heated oven as shown in Fig. 1(b). After crossing a 1D-OM, the isotopes A and B are deflected with different deflection angles because of different radiation pressure forces, which result from different detunings due to the isotope-shift effect.

As shown in Fig. 1(b), the atomic beam interacts with the tilted 1D-OM by an angle θ_0. With the absorption-emission cycle time on the order of 10^{-9} s, the atoms travelling inside the 1D-OM can absorb and emit photons many times, resulting in an average radiation pressure force. The atom velocity v can be decomposed into two orthogonal components, one is $v\cos\theta_0$ parallel to the molasses beams, and the other is $v\sin\theta_0$ perpendicular to the molasses beams. By adjusting the laser frequency to a value between two adjacent isotopes A's and B's resonance frequencies of the selected transition, two radiation pressure forces of two isotopes A and B could have the opposite signs to each other. For instance, the isotope A is subjected to a friction force and transversely decelerated and deflected from their original trajectories. However, the isotope B will be heated and deflected in a different direction. It is worth noting that the velocity component $v\cos\theta_0$ must be smaller than the capture velocity of the optical molasses for the efficient deflection.

The Yb atoms (atomic number $Z = 70$) have seven isotopes, i.e., two fermions (^{171}Yb, ^{173}Yb) with different nuclear spins ($I_{171} = 1/2$, $I_{173} = 3/2$) and five spinless bosons (^{168}Yb, ^{170}Yb, ^{172}Yb, ^{174}Yb, and ^{176}Yb). Corresponding to the $6s^2\ {}^1S_0 \rightarrow 6s6p{}^1P_1$ strong transition with a wavelength of $\lambda = 399$ nm, the Yb atoms have a high photon scattering rate. Its resonance frequency is defined as ω_0, and the natural linewidth is γ (~ 29 MHz). The relevant isotope shifts of the Yb atoms are shown in Fig. 2.

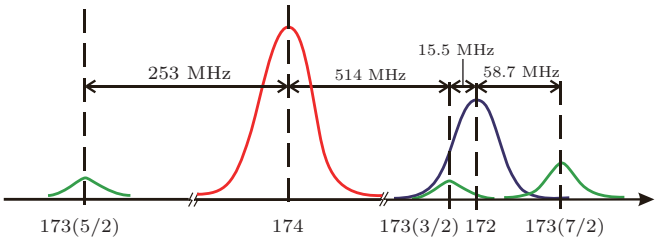


Fig. 2. (color online) Relevant isotope shifts of ^{174}Yb, ^{172}Yb, and ^{173}Yb for the transition $6s^2\ {}^1S_0 \rightarrow 6s6p{}^1P_1$ at the wavelength of 399 nm.

For ^{174}Yb, the resonance-frequency shifts from others are much larger than its own natural linewidth. This is very good for optically deflecting and selecting ^{174}Yb atoms from an atomic beam. In Fig. 1(b), a thermal Yb atomic beam effuses from the heated oven and then interacts with a pair of the counter-propagating laser beams at a crossing angle θ_0. The deflected atoms will be irradiated by the probe laser, and the induced fluorescence signal is detected by a photo-multiplier tube (PMT). The two linearly-polarized laser beams, whose polarizations are perpendicular to each other, each have a uniform intensity I and a diameter of Φ. The detuning of the laser frequency from the atomic resonance is given by $\Delta = \omega - \omega_0$, where ω is the angular frequency of the lasers. The saturation intensity and the spontaneous decay rate of the ${}^1S_0 \rightarrow {}^1P_1$ transition are $I_0 = \pi hc\Gamma/3\lambda^3 \approx 60\ \mathrm{mW/cm^2}$ and $\Gamma = 2\pi\gamma \approx 1.8 \times 10^8\ \mathrm{s^{-1}}$, respectively, where h is the Planck constant.[22]

4. Theoretical analysis

4.1. Deflection force

According to the Doppler cooling theory, two counter-propagating laser beams form a 1D-OM.[23] The radiation pressure forces $F_\pm$ of the two beams on the atoms are de-

scribed by

$$F_{\pm} = \pm\hbar k \frac{\Gamma}{2} \frac{I/I_0}{1+I/I_0+[2(\Delta \mp kv)/\Gamma]^2}, \tag{1}$$

where $\hbar$ refers to the reduced Planck constant, k denotes the wave vector of the molasses lasers, and v represents the instantaneous velocity along the laser beams. For the low intensity case, the atoms are subjected to a total force

$$\begin{aligned} F_{\text{sum}} &= F_+ + F_- \\ &= \hbar k \frac{\Gamma}{2} \frac{I}{I_0} \frac{kv}{\Gamma} 16\Delta/\Gamma \\ &\quad \times \left[\left(1+\frac{I}{I_0}\right)^2 + \frac{8}{\Gamma^2}\left(1+\frac{I}{I_0}\right)(\Delta^2+k^2v^2) \right. \\ &\quad \left. + \frac{16}{\Gamma^4}(\Delta^2-k^2v^2)^2 \right]^{-1}. \end{aligned} \tag{2}$$

In Eqs. (1) and (2), the Doppler effect has been taken into account. For the detuning $\Delta < 0$, the force F_{sum} always has the opposite sign to the velocity of atoms and behaves as a damping force. The atoms entering into the optical molasses with initial velocity v_0 will have a deflection angle θ. The capture velocity of the optical molasses is $v_c = +\Gamma/k \approx 11.5$ m/s. To guarantee that a substantial fraction of atoms have the transverse velocities within the capture range, a large angle θ_0 should be chosen.

4.2. Isotope separation of ^{174}Yb

We first discuss the isotope separation of ^{174}Yb atoms from the atomic beam. Several parameters are assumed reasonably as follows: $\Phi = 15$ mm and $\theta_0 = 60°$. The oven temperature is $T = 300$ °C. The atoms out of the collimating hole have a mean longitudinal (transverse) velocity about 311 m/s (11.5 m/s). For the sake of a good isotope separation, a considerable deflection angle should be achieved. Figure 3(a) shows the deflection angle θ versus saturation parameter I/I_0 for various initial velocities under the condition of $\Delta = -\Gamma/2$. With the increase of the molasses laser intensity, the deflection angle first increases and then levels off. The results show that the atoms with velocities less than 50 m/s can be completely deflected by a maximal angle of about 30°, where the optimum saturation parameter is about $I/I_0 = 1$. Figure 3(b) shows the dependence of the deflection angle θ on molasses laser detuning Δ for various initial velocities v_0 under the condition of $I/I_0 = 1$. With the increase of the absolute value of the laser detuning, the deflection angle of low-velocity atoms first increases sharply and then drops gently. Clearly, for the atoms with velocities less than 50 m/s, they will have similar deflection angles about 30° if the detuning is set at the any values between $-\Gamma$ and $-\Gamma/2$.

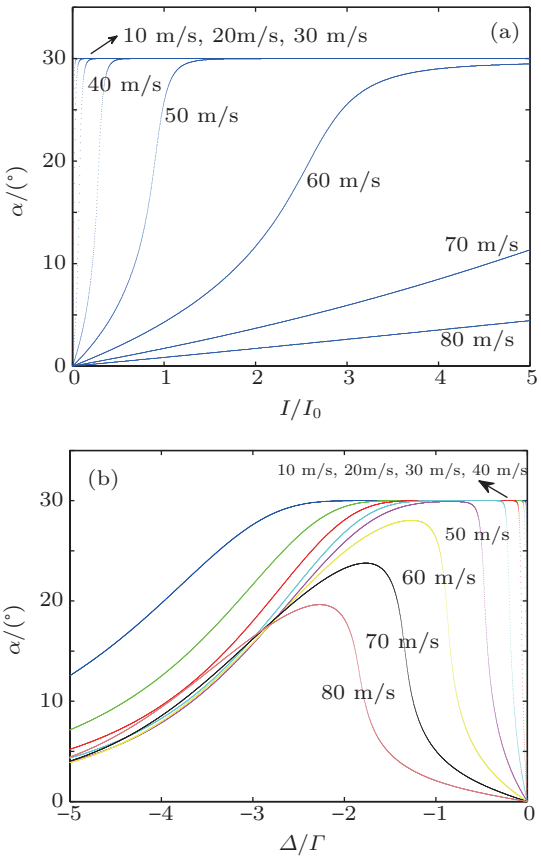


Fig. 3. (color online) (a) The ^{174}Yb deflection angle as a function of laser saturated parameter I/I_0 for various initial velocity v_0 (with detuning $\Delta = -\Gamma/2$). (b) The dependence of ^{174}Yb deflection angle on detuning Δ for various initial velocity v_0 (with saturated parameter $I/I_0 = 1$).

4.3. Isotope separation of ^{173}Yb from ^{172}Yb

As aforementioned, each Yb isotope has a different resonance frequency of the $^1S_0 \rightarrow {}^1P_1$ transition. For odd isotopes, there are hyperfine structures in the ground and the excited states. The transition used for selecting ^{173}Yb is the $^1S_0(F = 5/2) \rightarrow {}^1P_1(F' = 7/2)$ transition. Unfortunately, the ^{172}Yb transition overlaps with the hyperfine transitions from $F = 5/2$ to $F' = 3/2$ and F'=7/2 of ^{173}Yb as shown in Fig. 2. The isotope shift between ^{172}Yb and ^{173}Yb ($F' = 7/2$) is just about 58.7 MHz, so the peak of the ^{173}Yb ($F' = 3/2$) line is completely swamped in the peak of ^{172}Yb. The isotope separation among ^{172}Yb, ^{173}Yb ($F' = 3/2$), and ^{173}Yb ($F' = 7/2$) will be difficult.

The isotope ^{173}Yb atoms would partially experience the sub-Doppler cooling in the optical molasses because of the hyperfine structure.[24] However, Doppler cooling still dominates the process of cooling in this case. Therefore, our calculation is still based on the Doppler cooling theory. The molasses lasers are tuned at detuning Δ_1 relative to ^{172}Yb and Δ_2 relative to ^{173}Yb ($F' = 7/2$), respectively. After moving into the molasses beams, the two isotopes begin to separate from each other.

Similar to Eq. (2), the ^{172}Yb and ^{173}Yb atoms are respectively subjected to the following forces:

$$F_{\text{sum1}} = \hbar k \frac{\Gamma}{2} \frac{I}{I_0} \frac{kv}{\Gamma} \frac{16\Delta_1/\Gamma}{\left(1+\frac{I}{I_0}\right)^2 + \frac{8}{\Gamma^2}\left(1+\frac{I}{I_0}\right)(\Delta_1^2+k^2v^2) + \frac{16}{\Gamma^4}(\Delta_1^2-k^2v^2)^2}, \tag{3}$$

$$F_{\text{sum2}} = \hbar k \frac{\Gamma}{2} \frac{I}{I_0} \frac{kv}{\Gamma} \frac{16\Delta_2/\Gamma}{\left(1+\frac{I}{I_0}\right)^2 + \frac{8}{\Gamma^2}\left(1+\frac{I}{I_0}\right)(\Delta_2^2+k^2v^2) + \frac{16}{\Gamma^4}(\Delta_2^2-k^2v^2)^2}. \tag{4}$$

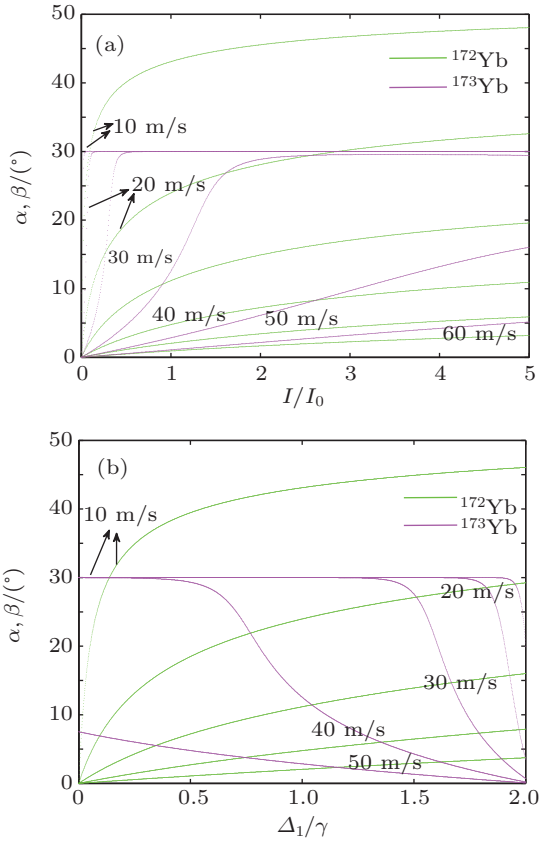


Fig. 4. (color online) (a) The ^{172}Yb and ^{173}Yb deflection angles each as a function of laser saturated parameter I/I_0 for various initial velocity v_0 (with detuning $\Delta_1 = \gamma$). (b) The dependences of ^{172}Yb and ^{173}Yb deflection angles on detuning Δ_1 for various initial velocity v_0 (with saturated parameter $I/I_0 = 1$).

Here, F_{sum1} (F_{sum2}) is antiparallel (parallel) to the x-axis direction for $\Delta_1 > 0$ and $\Delta_2 < 0$, and F_{sum1} behaves as a heating force, while F_{sum2} turns out to be a viscous force. The ^{172}Yb atoms move to the left of the initial velocity direction, indicating that they have been heated. However, the ^{173}Yb atoms are cooled and deflected to the right. Both isotopes with large velocities will be undeflected. Now we will discuss the optimum laser detuning and intensity for the isotope separation of ^{172}Yb and ^{173}Yb. As shown in Fig. 1(b), to separate these two isotopes well, the two angles α and β should be large enough. At first, we assume laser detuning $\Delta_1 = \gamma$, then $\Delta_2 = \gamma - 58.7$ MHz. In Fig. 4(a), when the laser intensity is $I \sim 2I_0$, the ^{173}Yb atoms with velocities less than 40 m/s have a deflection angle $\alpha \approx 30^\circ$. However, the angle α decreases dramatically as the velocity increases. The deflection angle β of ^{172}Yb is about 45° when the velocity is 10 m/s, and then drops faster than that of ^{173}Yb when the velocity is greater than 20 m/s. For both isotopes, the deflection angles become very small when the velocity is larger than 60 m/s. According to these results, the laser intensity will be set to $I \sim I_0$ for an efficient isotope separation.

With $I/I_0 = 1$, the dependences of the deflection angle on the laser detuning with various velocities of the atoms are shown in Fig. 4(b). Since the isotope shift between isotopes ^{172}Yb and ^{173}Yb is about 58.7 MHz, the detuning Δ_1 cannot exceed this value. Figure 4(b) implies that Δ_1 could be around γ, so the ^{173}Yb atoms can be separated efficiently from ^{172}Yb.

4.4. Estimation of separation efficiency and purity

At present, the 399-nm laser linewidth is typically around 1 MHz.[25,26] It is small enough compared with the isotope shift for possible isotope separation. In order to estimate the efficiency and purity of isotope separation, the atomic beam divergence should be taken into account. The separation efficiency represents the fraction of the desired isotopic component B that can be deflected from the total isotope B entering into the separation zone. To obtain the maximum deflection angle, the atoms need to absorb an average number of photons

$$N_0 \approx m v_{0\max} \cos(\theta_0 - \theta_{\text{d}}/2)\lambda/h, \tag{5}$$

where $v_{0\max}$ denotes the maximum initial velocity with which the atoms can be completely deflected. Among the Yb atomic transitions, the $^1\text{S}_0 \rightarrow {}^1\text{P}_1$ transition is not closed. The atoms can decay from $^1\text{P}_1$ to $^3\text{D}_2$ or $^3\text{D}_1$ state, then to lower $^3\text{P}_0$, $^3\text{P}_1$, and $^3\text{P}_2$ states. Atoms at $^3\text{P}_0$ and $^3\text{P}_2$ metastable states will not quickly return to the ground state. Thus, the $^1\text{P}_1$ state has a probability ξ_0 of returning to the ground state and a probability ξ_1 of decaying to the metastable states. The efficiency is[27]

$$\eta = \int_0^{v_{0\max}} g(v)\,\text{d}v \int_{N_0}^{+\infty} \xi_0^N \xi_1 \,\text{d}N, \tag{6}$$

where $g(v)$ is the normalized longitudinal velocity distribution. Since θ_{d} is much smaller than θ_0 and ξ_1 is on the order of 10^{-7},[28] the efficiency is mainly limited by the broad longitudinal velocity distribution.

In the case of separating ^{174}Yb, $v_{0\max} \approx 50$ m/s and $N_0 \approx 4350$. If the atoms are not decelerated along the atomic

beam direction, $g(v)$ is replaced by $f(v)$ and the calculated efficiency is 0.1%. For the ^{173}Yb separation, the efficiency is just 0.01% due to the low velocity $v_{0\max} \approx 30$ m/s. On the other hand, because the isotope shift between ^{172}Yb and ^{173}Yb is comparable to the natural linewidth, the separated ^{173}Yb atomic beam may be contaminated by some ^{172}Yb atoms, which will reduce the purity by 16% (maximum).

4.5. Improvement in separation efficiency

We may obtain a larger deflected atom flux by increasing the interaction time, i.e., the molasses beam diameter. However it is limited by the available laser power due to the optimal condition $I \approx I_0$. The isotope separation efficiency and atomic flux could be increased by taking the following measures: (i) further compressing the divergence of the atomic beam by using a two-dimensional optical molasses (2D-OM) perpendicular to the atomic beam; (ii) reducing the longitudinal velocity by using a Zeeman slower or a similar technology; (iii) adding another compression stage after the Zeeman slower.[29,30] For instance, with the help of the Zeeman slower and 2D-OM, typically, the mean longitudinal velocity can be reduced from 300 m/s to 20 m/s with a narrow velocity spread.[21] According to our calculation, in this case, the separation efficiency could be close to 100%.

5. Conclusion

We theoretically analyze the Yb isotope-separating process with the 1D-OM formed by two counter-propagating laser beams. The results show that for the atoms with velocities less than $v_{0\max}$, the deflection angle is independent of the atom velocity and the laser intensity for the given detuning. By adjusting the molasses laser detuning, various Yb isotope atoms can be seperated from the initial atomic beam and form a purified single-isotope continuous atomic beam with a good collimation. Furthermore, we propose a scheme to improve the separation efficiency and purity by combining with the Zeeman slowing and 2D-OM techniques. Our theoretical calculations confirm the experimental results presented in Ref. [2] and predict that even more and much purer isotopes may be obtained under the optimal conditions described in this paper. Our findings will give a complete understanding of the isotope separation with the beam deflection method and a helpful guideline for simply obtaining pure isotopes of various elements.

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