Design of magnetic system to produce intense beam of polarized molecules of H\textsubscript{2} and D\textsubscript{2}

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Abstract. A magnetic-separating system is designed to produce polarized molecular high-density beams of H\textsubscript{2}/D\textsubscript{2}. The distribution of the magnetic field inside the aperture of the multipole magnet was calculated using the Mermaid software package. The calculation showed that the characteristic value of the magnetic field is 40 kGs, the field gradient is about 60 kGs/cm. A numerical calculation of the trajectories of the motion of molecules with different spin projections in this magnetic system is performed. The article discusses the possibility of using the magnetic system designed for the creation of a high-intensity source of polarized molecules. The expected intensity of this source is calculated. The expected flux of molecules focused in the receiver tube is $3.5 \times 10^{16}$ mol/s for the hydrogen molecule and $2.0 \times 10^{15}$ mol/s for the deuterium molecule.

1. Introduction

The existing sources of polarized hydrogen and deuterium atoms make it possible to obtain beams with an intensity of about $10^{17}$ atoms/s. A detailed review of the existing sources of polarized hydrogen atoms is given in [1, 2]. These sources are based on the spin-separation method. This principle can also be used for the production of polarized molecules. Thus, hydrogen molecules having different projections of the nuclear magnetic moment can be spatially separated in an inhomogeneous magnetic field, which was first demonstrated in Ref. [3].

We previously demonstrated [4, 5, 6] the production of polarized molecules of hydrogen/deuterium using the existing atomic beam source of polarized deuterium atoms [7]. In this source, superconducting sextupole magnets were used for the spatial separation of molecules with different nuclear spin projections. The experimentally measured flux of polarized molecules with a negative nuclear spin projection focused into the receiving detector tube was found to be $Q_{\text{tube} H_2} = 1.8 \cdot 10^{12}$ mol/s for the hydrogen molecules and $Q_{\text{tube} D_2} = 3.8 \cdot 10^{11}$ mol/s for the deuterium molecules.

These intensities can be increased by orders of magnitude if all linear dimensions of the experimental setup and magnets will be up-scaled, for example, by a factor of 10 [8]. This article discusses the possibility of creating this type of molecular source and its expected intensity.

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2. Simulation of the spin separating magnet.

In a new source, a 60-pole magnet for spin separation of molecules should be used with the inner bore of 400 mm. An increase in the number of poles of the magnet will make it possible to obtain the larger gradient of the magnetic field, with the same value of the magnetic field at the poles, and, thereby, to increase the deflection force.

The geometry of the 1/60 part of such a developed magnet is shown in Figure 1. The area of the coil with current is $S_{\text{coil}}=3.92$ cm$^2$, the current density passed through the coil can reach $j=100$ kA/cm$^2$, the total current, respectively, is up to $I=392$ kA.

![Figure 1. The geometry of a 60-pole magnet. Dimensions are in (mm). The following areas are highlighted: aperture of vacuum chamber – blue color, coil with current – red color, iron heel – green color](image1)

The magnetic field distribution $B(r,\phi)$ in the inner aperture of the magnet was calculated by Mermaid software package (developed by BINP). The distribution of $B(r,\phi)$ is shown in Figure 2. It can be seen that the field and, consequently, its gradient is maximal near the pole of the magnet.

![Figure 2. The magnetic field distribution $B(r,\phi)$ in the vacuum chamber region, created by a 1/60 part of the magnet. The distribution is obtained as a result of computer simulation](image2)

The simulation showed that the characteristic value of the magnetic field at the magnet pole at $r=200$ mm is $B=40$ kGs, the field gradient near the pole is about $\nabla B=60$ kGs/cm.

3. Prototype of the experimental setup

For the spatial separation of molecules with a specific projection of the nuclear spin, the following geometry of the installation prototype was proposed, which is shown in Figure 3. Molecules with different projections of the nuclear spin are emitted from the nozzle of the source, whose internal diameter is 380 mm, the outer diameter is 400 mm (width of the nozzle, respectively, is 10 mm; the nozzle area is 122 cm$^2$, which is approximately $10^3$ greater than the area of the nozzle used before). The distance from the nozzle to the entrance of the focusing 60-pole magnet is 1000 mm. The length of the magnet is 2000 mm. At the entrance of the magnet a disk is placed with a diameter of 380 mm, forming an annular diaphragm, an outer diameter is 400 mm and a width is 10 mm. With such a geometry the molecules are moving in the magnet in the vicinity of the poles, where the field gradient and, consequently, the deflection force, are maximal. The magnet has a linearly converging aperture, such that the output diameter of the magnet is 370 mm. At a distance of 500 mm from the end of the magnet, along with the axis of the installation, a receiver for molecules is placed, with a diameter of 330 mm. It contains a turbopump for compressing a polarized gas. In such a geometry the direct ballistic flux of molecules cannot reach a receiver.

To determine the fraction of molecules with different spin projections that move out of the magnet from the total number of molecules from the source nozzle, a Monte Carlo computer program was developed to simulate the motion of neutral particles in installations with cylindrical geometry in the presence of an inhomogeneous magnetic field. The program takes into account of Maxwell's particle velocity dispersion, the flow distribution from the nozzle according to the cosine law, the dependence
of the magnetic moment for each quantum state of the molecule on the magnitude of the magnetic field, the unit coefficient of adhesion of molecules to the surface of the vacuum chamber. In the simulation, in-beam scattering is not taken into account. The magnetic field is given as a table of numbers from Mermaid simulation. The trajectories were calculated for a hydrogen molecule with a nozzle temperature $T=8\text{K}$ and for a deuterium molecule with $T=11\text{K}$ (below this temperature molecular deuterium condensates).

![Diagram of the prototype installation](image)

**Figure 3.** The geometry of the prototype installation. Dimensions are in (mm). The blue line shows one of the possible trajectories of molecules, which, being focused by the magnetic field, will enter the molecular receiver.

4. **Computer simulation of molecules motion**

The results of computer simulation of the movement of molecules in the prototype of installation are given below.

Table 1 contains simulation results for the ratio of the number of molecules with different spin projections at the exit from the magnet to the total number of molecules from the source nozzle and the polarization. Here we use the notation: $N_{\text{positive}}$ is the number of molecules with a positive effective magnetic moment (negative nuclear spin projection $m_I=-1$, focusing), $N_{\text{zero}}$ is the number of molecules with zero spin projection (free or ballistic motion, $m_I=0$), $N_{\text{negative}}$ is the number of molecules with negative effective magnetic moment (positive nuclear spin projection $m_I=+1$, defocusing), $N_{\text{all}}$ is total number of molecules with all possible spin projections.

**Table 1.** Simulation results: the ratio of the number of molecules with different projections of nuclear spin and polarization at the exit from the magnet to the total number of molecules from the nozzle

| molecule | $N_{\text{positive}} / N_{\text{nozzle}}$ | $N_{\text{zero}} / N_{\text{nozzle}}$ | $N_{\text{negative}} / N_{\text{nozzle}}$ | $N_{\text{all}} / N_{\text{nozzle}}$ | $P_z$ |
|----------|------------------------------------------|----------------------------------------|------------------------------------------|-----------------------------------|------|
| $H_2$    | $6.31\cdot10^{-5}$                      | $7.66\cdot10^{-6}$                     | $6.78\cdot10^{-8}$                      | $7.08\cdot10^{-5}$               | -0.88 |
| $D_2$    | $1.87\cdot10^{-5}$                      | $6.04\cdot10^{-6}$                     | $2.44\cdot10^{-6}$                      | $2.72\cdot10^{-5}$               | -0.59 |

In Table 2, the same ratios are given, only for molecules that fall into the receiver.

**Table 2.** Simulation results: the ratio of the number of molecules with different projections of nuclear spin and polarization in the receiver to the total number of molecules from the nozzle

| molecule | $N_{\text{positive}} / N_{\text{nozzle}}$ | $N_{\text{zero}} / N_{\text{nozzle}}$ | $N_{\text{negative}} / N_{\text{nozzle}}$ | $N_{\text{all}} / N_{\text{nozzle}}$ | $P_z$ |
|----------|------------------------------------------|----------------------------------------|------------------------------------------|-----------------------------------|------|
| $H_2$    | $4.60\cdot10^{-5}$                      | 0                                      | 0                                        | $4.60\cdot10^{-5}$               | -1.0 |
| $D_2$    | $3.83\cdot10^{-6}$                      | 0                                      | 0                                        | $3.83\cdot10^{-6}$               | -1.0 |
From the analysis of the tables, it can be seen that the geometry of the projected installation is chosen in such a way that only molecules with a negative projection of the nuclear spin $m_I$ = -1 enter the receiver tube. It is clear that the aperture of the magnet was chosen to be converging, so that the molecules with the projection of the spin $m_I$ = 0, +1 hit the walls of the vacuum chamber and pumped out. It can be seen from Table 1 that the fraction of these molecules at the exit of the magnet is the order of magnitude smaller than the molecules with $m_I$ = -1.

Knowing the fraction of molecules that enter into the receiver tube from the total flow from the nozzle, one can estimate the expected flow of molecules into the receiver tube. For hydrogen molecules, the expected flux is $Q_{tube \text{H}_2} = 3.5 \cdot 10^{16}$ mol/s and for the deuterium molecule $Q_{tube \text{D}_2} = 2.0 \cdot 10^{15}$ mol/s. A comparison of the flow of molecules focused in the receiver between existing BINP SB RAS source and the prototype source is given in Table 3.

### Table 3. Comparison of the flow of molecules focused in the receiver tube for an existing (BINP) and projected source prototype

| molecule | existing source in the BINP (experiment) | prototype source (simulation) |
|----------|------------------------------------------|-------------------------------|
| H$_2$    | $1.8 \cdot 10^{12}$ mol/s                | $3.5 \cdot 10^{16}$ mol/s    |
| D$_2$    | $3.8 \cdot 10^{11}$ mol/s               | $2.0 \cdot 10^{15}$ mol/s    |

It can be seen that the gain when using a prototype source is about $10^4$ for a hydrogen molecule and $10^5$ for a deuterium molecule.

### 5. Conclusion

The magnet system of the new source to produce an intense beam of polarized molecules of hydrogen isotopes has been suggested. The field of a 60-pole magnet and the trajectory of molecules in this large installation are calculated. The calculations have shown that the intensity of the developed molecular source may exceed available at BINP source by more than $10^4$ for the hydrogen molecules and more than $10^3$ for the deuterium molecules.

The resulting high-intensity polarized molecular beams can be used for future accelerator experiments and as a possible fuel for fusion reactors [9].

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