The influence of interatomic collisions on the angular distribution of Cs atomic flow from microchannel

A Yu Rumyantsev1, M V Petenko1,2, S A Poniaev2,3, Yu A Shustrov2, V P Kochegarov4 and D L Schennikov1

1 Russian Institute of Radionavigation and Time, 120 Obukhovskoy Oborony prospect, St. Petersburg, 192012, Russia
2 Ioffe Institute, 26 Politekhnhcheskaya Street, St. Petersburg, 194021, Russia
3 Mozhaisky Military Space Academy, 13 Zhdanovskaya Street, St. Petersburg, 197198, Russia

E-mail: m.petenko@mail.ioffe.ru, s.poniaev@gmail.com

Abstract. Beams of alkali atoms are typically used in precise quantum devices, such as atomic beam frequency standards. In order to know more exactly parameters of atomic beam tubes and frequency standards (frequency instability), it is necessary to investigate the propagation of Cs atoms after the channel exit. In this work theoretical calculations of angular distribution of Cs atomic flow from a microchannel are carried out. The Monte-Carlo direct numerical simulation of Cs atom propagation is also performed to estimate the influence of interatomic collisions on the atomic flow.

1. Introduction
Alkali atoms are typically used in precise quantum devices, such as frequency standards based on alkali vapour cells [1,2] or atomic beam tubes [3], and quantum magnetometers with optical pumping [4,5]. Beams of Cs atoms with temperature in the range of 100 – 130°C are used in atomic beam frequency standards. These beams outflow from microchannels with typical length-to-diameter ratios of 50 – 200. In order to know more exactly parameters of atomic beam tubes and frequency standards (frequency instability), it is necessary to investigate the propagation of Cs atoms after the channel exit. Nowadays theoretical calculations are widely used to describe Cs atomic flow [3], but the influence of interatomic collisions on the atomic flow is not taken into account in these calculations.

In this work theoretical calculations of angular distribution of Cs atomic flow from a microchannel are carried out. The Monte-Carlo direct numerical simulation of Cs atom propagation is also performed to estimate the influence of interatomic collisions on the atomic flow.

2. Results of theoretical calculations
The propagation of Cs atoms is investigated by using a microchannel with the following parameters: channel length \( L = 1 \text{ cm} \), channel diameter \( d = 50, 100 \) and \( 200 \mu \text{m} \). The scheme of the flow is presented in figure 1. The input volume contains Cs vapor with temperature \( T = 120 \) °C, so the free path of Cs atoms takes on a value \( \lambda = 0.066 \text{ cm} \) since the cross-section of Cs atom interatomic collisions is \( \sigma = 2.35 \times 10^{-13} \text{ cm}^2 \) [6]. The pressure of Cs vapor in the input reservoir takes on a value
Figure 1. Scheme of Cs atom flow through microchannel.

$P_{Cs} = 1.85 \times 10^3$ Torr, and Knudsen number is $Kn_{L} = \lambda / L = 0.066$. After the propagation through the microchannel Cs atoms flow into vacuum and the angular distribution of the atomic flow is described by the function $J(\theta)$.

It is necessary to note that the increase in the channel length to the values that exceed the free path of Cs atoms in the input volume leads to an essential influence of interatomic collisions on the atom propagation inside the channel and on the angular distribution of the atomic flow after the channel. In our work we used the theoretical model [7] in which the atom-wall interaction obeys the law of diffuse reflection and the atom scattering due to interatomic collisions is taken into account.

The angular distribution of Cs atomic flow at the microchannel exit is defined by

$$J(\theta) = \frac{\dot{N}}{\pi K} j(\theta), \quad (1)$$

where $J(\theta)$ is the intensity of the atomic flow in atoms·s$^{-1}$·Sr$^{-1}$ at a polar angle $\theta$ from the tube axis, $\dot{N}$ is the total flow rate through the channel, $K$ is the transmission probability and $j(\theta)$ is the angular distribution function. Since the gas in the input volume is Maxwellian, the total atomic flow rate through the channel is defined by the Cs vapor characteristics in the input reservoir and by the channel parameters

$$\dot{N} = K \left( \frac{n\bar{v}}{4} \right) \left( \frac{\pi d^2}{4} \right), \quad (2)$$

where $n$ is the number density of Cs atoms in the source, and $\bar{v}$ is the mean speed of the atoms. Since the integral of $J(\theta)$ over the front hemisphere must be equal to the total flow rate, $K$ and $j(\theta)$ are related by

$$K = 2 \int_{0}^{\pi/2} j(\theta) \sin \theta \, d\theta. \quad (3)$$

The calculation of the angular distribution of the atomic flow from different microchannels was carried out with and without taking into account interatomic collisions. The calculation was performed by using the expressions for the function $j(\theta)$ which are defined in [7,8]. The parameters of the calculation in the collisionless case corresponding to the calculation performed in [3,9] were chosen.
The results of the calculation are shown in figure 2. In the graphs the solid lines show the angular distributions in which interatomic collisions are taken into account, and the dashed line is for the collisionless case. It follows from the results obtained in the calculations that the consideration of interatomic collisions in the description of the propagation of atoms leads to a reduction in the atomic flow in the axial (central) part of the atomic flux in 2.5 – 3 times depending on the channel geometry. The angular distribution becomes flatter and exceeds the distribution obtained without taking into account interatomic collisions for large angles $\theta$.

**3. Results of numerical simulation**

The numerical simulation was performed by the DSMC method [10] using the OpenFOAM software package [11]. The calculations were performed for collision and collisionless flows. The variable hard sphere (VHS) model was employed [12,13] for simulation of collision flows.

The interaction of the sample particles with the channel walls was calculated in the diffuse approximation, i.e., as a reflection with adhesion. The direction of the reflected particles was determined by the cosine law, and their speeds were randomly chosen on the basis of the maxwellian thermal distribution of velocities at the temperature equal to the temperature of the channel walls. In our simulation the temperature of the channel wall was taken to be 120 °C.

![Figure 2](image-url)
The angular distribution of the Cs atom flow was calculated by using the number of sample particles passing through a unit area at angle $\theta$. The number of sample particles was time-averaged over the period from 0.05 s to 0.1 s from the flow start. The results are shown in figure 3. The red curve show results of numerical simulation, the black curve show results of theoretical calculations for comparison, the solid lines are angular distributions obtained with interatomic collisions taken into account, the dashed lines were obtained for the collisionless case. It can be seen from figure 3 that the results of numerical simulation are in good agreement with the results of theoretical calculations. The behavior of the angular distributions in the axial region of atomic beam obtained numerically can be explained by the statistical errors, taking into account the limited number of sample particles passing through the unit area in the axial region. These flows of atoms obtained numerically are quantitatively lower than the theoretical values.

Table 1 shows the values of total flow rate through the channel in case of interatomic collisions are taken into account. The values $N_{\text{ah}}$ and $N_{\text{num}}$ represent the flow of atoms through the channel, calculated by analytical formulas and by numerical simulation respectively.
4. Conclusion

The values of the total flow rate of atoms from the channel obtained in numerical simulation are lower than the theoretical rates in 1.35 – 1.69 times, depending on the channel geometry. The difference can be explained by using a fairly simple calculation model of diffuse law of interaction of atoms with the channel walls. Further investigations are necessary to model a more complex interaction of the particles with the walls, in particular taking into account the direction and speed of the particles before the interaction.

Results of numerical simulation are in good agreement with theoretical calculations. This agreement allows the use of analytical formulas in the description of the spread of the atoms from the channel in the case of a simple geometry of the system, for example in the case of a single cylindrical channel. In the case of more complex geometrical systems, such as a channel with a square cross-section or multichannel collimator, the result obtained by using analytical formulas can have a significant divergence with the results of numerical simulation and with the real physical process.

The angular distributions of Cs atomic flow obtained in our work by using numerical simulation and analytical formulas show a significant influence of interatomic collisions inside a channel on the atomic flow. If interatomic collisions are taken into account, a significant decrease (in 2.5 – 3 times) of the atomic flow rate in the axial (central) region of the beam results. Since the central region of the atomic beam is used in the atomic beam frequency standards, it is necessary to consider interatomic collisions when describing the propagation of cesium atoms from microchannels.

References
[1] Ermak S V, Petrenko M V and Semenov V V 2016 Tech. Phys. Lett. 42 127
[2] Fedorov M I, Ermak S V, Petrenko M V, Pyatyshev E N and Semenov V V 2016 J. Phys.: Conf. Ser. 769 012046
[3] Pimenov A V and Pleshanov S A 2010 Electronnaya Tekhnika. SVCH Tekhnika 507 16 (in russian)
[4] Baranov A A, Ermak S V, Sagitov E A, Smolin R V and Semenov V V 2016 Tech. Phys. Lett. 42 186
[5] Sagitov E A, Ermak S V, Petrenko M V and Semenov V V 2016 J. Phys.: Conf. Ser. 769 012044
[6] Vanier J and Audoine C 1989 The quantum physics of atomic frequency standards (Philadelphia: IOP Publishing Ltd) p 453
[7] Olander D R and Kruger V 1970 J. Appl. Phys. 41 2769
[8] Lucas C B 2014 Atomic and Molecular Beams. Production and Collimation (New York: CRC Press) p 211
[9] Beijerinck H C W and Verster N F 1975 J. Appl. Phys. 46 2083
[10] Bird G A 1994 Molecular gas dynamics and the direct simulation of gas flows (Oxford: Clarendon)
[11] OpenFOAM®, www.openfoam.com
[12] Bird G A 1978 Annu. Rev. Fluid Mech. 10 11
[13] Bird G A 1983 Phys. Fluids 26 3222