Studies on Beam Formation in an Atomic Beam Source

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Abstract. Atomic beam sources (ABS) are widely used workhorses producing polarized atomic beams for polarized gas targets and polarized ion sources. Although they have been used for decades the understanding of the beam formation processes is crude. Models were used more or less successfully to describe the measured intensity and beam parameters. ABS's are also forseen for future experiments, such as PAX [1]. An increase of intensity at a high polarization would be beneficial. A direct simulation Monte-Carlo method (DSMC) [2] was used to describe the beam formation of a hydrogen or deuterium beam in an ABS. For the first time a simulation of a supersonic gas expansion on a molecular level for this application was performed. Beam profile and Time-of-Flight measurements confirmed the simulation results. Furthermore a new method of beam formation was tested, the Carrier Jet method [3], based on an expanded beam surrounded by an overexpanded carrier jet.

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MOTIVATION

Polarized ABS's are utilized to provide nuclear-polarized atomic hydrogen (H) and deuterium (D) beams. H_2 or D_2 gas is dissociated and the atomic gas expands through a cooled nozzle into the vacuum. A beam of high brightness is then formed by a skimmer and a collimator to adapt the beam to the acceptance of the subsequent system of sextupole magnets. Based on the Stern-Gerlach principle, these magnets focus (defocus) atoms with electron-spin projection +1/2 (-1/2) along the magnetic field within the magnet bores. The electron-spin polarized beam then enters a rf transition unit, which changes the nuclear polarization by inducing transitions between the hyperfine states. To achieve a high output intensity, the atomic beam has to fulfill several requirements like high flow rate, low transversal and longitudinal temperature, and a high degree of dissociation α. The pressure within and at the exit of the nozzle corresponds to the transition region between laminar and molecular flow. There, the use of continuum-flow models is of restricted validity. Thus, a DSMC method [2] was used to describe the processes during gas expansion.

SUPERSONIC GAS EXPANSIONS AND DSMC

A free-jet atomic or molecular beam can be produced by a supersonic gas expansion from a high-pressure gas source (temperature T_0) into a low pressure background. As a

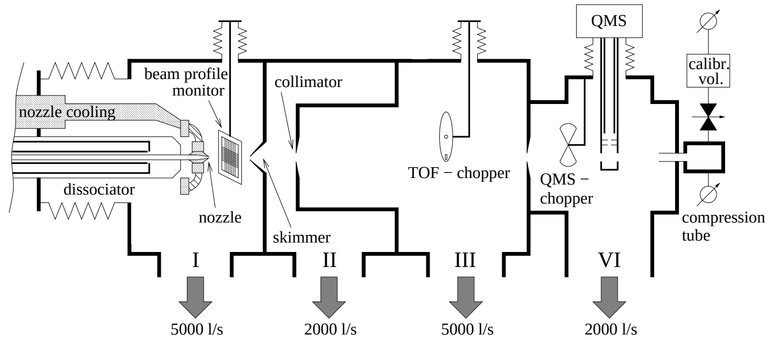

FIGURE 1. The experimental setup.

result of the pressure difference the gas is accelerated. From energy considerations the maximum or terminal velocity can be derived:

$$v_\infty = \sqrt{\frac{2k_\mathrm{B}}{m}\left(\frac{\gamma}{\gamma-1}\right)T_0}, \tag{1}$$

with the particle mass m, $\gamma = c_\mathrm{p}/c_\mathrm{V}$ and the Boltzmann constant k_B. For a pure atomic (molecular) hydrogen expansion $v_\infty = 2031\,(1436)$ m/s.

The DSMC method [2] is a technique for the computer modeling of a real gas by some thousands or millions of simulated particle trajectories. The velocity components and position coordinates of these particles evolve in time as the particles are concurrently followed through representative collisions and boundary interactions. The decoupling of the motion and collisions of the particles over small time steps and the division of the flow field into small cells are the key computational assumptions associated with the DSMC method. The time step should be much smaller than the mean collision time and a typical cell dimension should be much smaller than the local mean free path. For our purpose the geometry of the beam forming elements nozzle, skimmer, and collimator are implemented as boundary walls with temperature T (see Fig. 2).

THE EXPERIMENTAL SETUP

An atomic beam test stand (ABT) had been set up and equipped with several diagnostic devices (Fig. 1). A microwave dissociator [4] mounted on the first chamber produces H or D. α is determined with the quadrupole mass spectrometer (QMS). The velocity distribution of the particles in the atomic beam is determined with the time-of-flight (TOF) method. A fast chopper cuts a small bunch of particles out of the beam, and their arrival time at the QMS is measured. Since the particles have different velocities, a TOF distribution $F(t)$ is measured. By deconvolution the effects of the opening function of the chopper wheel and the electronics could be removed and the translational beam temperature $T_\mathrm{tr,x}$ and the mean velocity v_x in beam direction could be determined. A beam-profile monitor [5] is used to measure intensity profiles of the atomic hydrogen or deuterium beam.

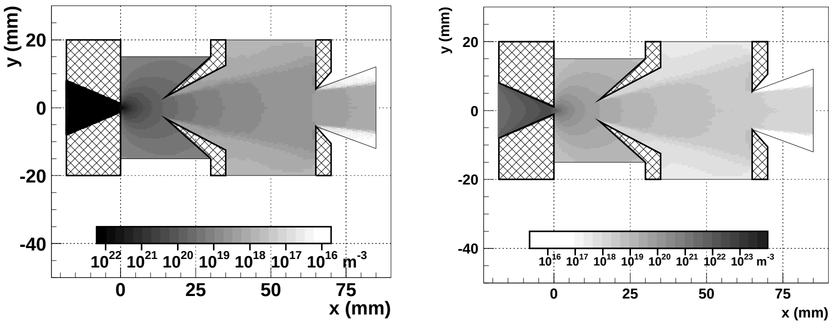

FIGURE 2. Calculated density distribution for a H_2 expansion (left) and the atomic part of a H/H_2 expansion (right, $\alpha = 0.63$) with a nozzle throughput of 1 mbar$l$/s and a nozzle temperature of 100 K.

TABLE 1. Comparison of the calculated and measured parameters of (i) a pure molecular and (ii) a partly dissociated hydrogen beam. For the partly dissociated beam $\alpha = 0.63$.

		v_x (m/s)	$T_{tr,x}$ (K)
molecular beam	measurement	$1274 \pm 8 \pm 13$	$19.0 \pm 1.1 \pm 0.9$
	simulation (original)	$1334 \pm 12\,^{+5}_{-15}$	$33.3 \pm 1.6\,^{+0}_{-3}$
	simulation (Ref. [6])	$1371 \pm 2\,^{+5}_{-15}$	$19.0 \pm 0.2\,^{+0}_{-3}$
	atoms		
partly dissociated beam	measurement	$1750 \pm 47 \pm 24$	$25.7 \pm 4.9 \pm 1.5$
	simulation	$1760 \pm 20\,^{+6}_{-19}$	$41.0 \pm 3.4\,^{+0}_{-3}$
	molecules		
	measurement	$1579 \pm 51 \pm 17$	$23.7 \pm 7.1 \pm 1.0$
	simulation	$1590 \pm 33\,^{+6}_{-17}$	$44.0 \pm 4.3\,^{+0}_{-3}$

SIMULATION RESULTS AND EXPERIMENTAL VERIFICATION

DSMC simulations of expansions of H_2 and partially dissociated hydrogen were performed. The calculated particle-density distribution of a H_2 and a H expansion is shown in Fig. 2. The density near the nozzle follows a $\cos(\theta)$ distribution. Skimmer and collimator form a low-diverging and sharp-bound molecular beam. In Tab. 1, v_x and $T_{tr,x}$ are compared as they result from measurement and DSMC calculation. The calculated v_x is close to the measured one, but $T_{tr,x}$ is appreciably too high. The problem was studied [6] and it was found that $T_{tr,x}$ contrary to v_x, strongly depends on the parameters of the collision processes used in the DSMC. It seems that certain parameters, chosen by the editors of the used simulation code, are not fully correct for the low-T region.

Energy considerations showed a discrepancy between expected and measured beam parameters of partially dissociated hydrogen beams. This finding would be explained by the assumption that T_0 is higher than T_{nozzle}, i.e., that the gas does not reach the thermal equilibrium. This explanation was confirmed by DSMC calculations.

The data, obtained by the DSMC calculations for a partly dissociated hydrogen beam, could be further compared with the results of beam-profile measurements, made with the beam-profile monitor. Fig. 3 shows the calculated distribution of the resistances

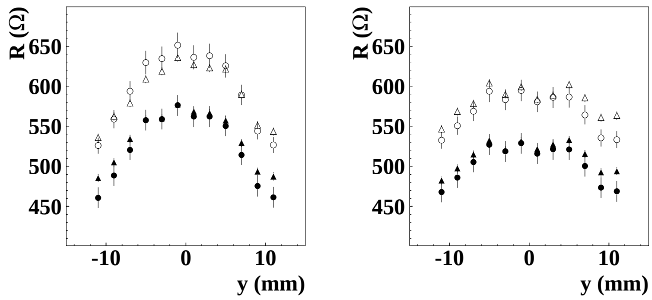

FIGURE 3. Comparison of the calculated (circles) and measured (triangles) distributions of the wire resistances at distances between wire plane and nozzle exit of 10 mm (left-hand side) and 20 mm (right-hand side). The nozzle throughput was 1 mbar*l*/s (full symbols) and 2 mbar*l*/s (open symbols).

compared with the measured one. Both distributions are not smooth due to the variations in the response functions of the wires but in good agreement.

The carrier jet method was proposed [3] to increase the phase-space density of the atomic beam and thus to reach a higher intensity through the collimator of the ABS. An over-expanded carrier jet, surrounding the inner atomic beam, was predicted to cool and to confine the inner beam. The mixing of the two gases has to be small and the carrier gas has to be removed by the skimmer and pumped away. The predicted carrier-jet effect could not be observed for H and D at the operational parameters of the ABS. It was, however, observed for an Ar beam surrounded by a N_2-carrier jet. Both experimental findings are consistent with the results of DSMC calculations.

SUMMARY AND OUTLOOK

It has been shown that the DSMC method is an excellent tool to describe the processes occurring in the expansion of light and also heavier gases in the transition region between laminar and molecular flow [7]. The results of the calculations were confirmed by the measurements, performed at an ABT. The origin of the discrepancies between simulated and measured temperatures was found, the problem could be explained by the influence of the input parameters of the DSMC code. The method could be used to design a new generation of ABS's by implementation of sextupole magnets into the DSMC code to finally understand the behavior of the output intensity of an ABS.

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