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Computer simulation and visualization of supersonic jet for gas cluster equipment

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ABSTRACT

Supersonic nozzle is a key component of a gas cluster condensation system. We describe a flow visualization system using glow discharge with annular or plane electrodes. The geometric parameters of a supersonic jet under typical conditions used in a gas cluster ion beam accelerator are investigated. As well numerical simulations were performed. Dependence of inlet and ambient pressures and nozzle throat diameter on the shock bottle dimensions is described for different working gases. Influence of condensation rate on shock bottle axial size is discussed.

1. Introduction

Recent decades, gas cluster ion beams (GCIB) have been under extensive study. GCIB are widely used in practical applications, such as precise surface polishing and etching, ultra-shallow implantation, ion-assisted deposition of thin films, probing in SIMS technique [1–3], as well as in investigations of fundamental properties of matter [4,5].

The usual way of obtaining gas clusters is adiabatic expansion of a working gas through a supersonic nozzle, so that expanded gas becomes cold enough for clusterization. Information on properties of the jet below a nozzle is essential for optimization a nozzle and skimmer geometry and the distance between them.

The typical structure of a supersonic jet shown in Fig. 1 is described in [6,7]. It is shown in Fig. 1, that the gas expanding to the ambient pressure p_∞ forms a “shock bottle” configuration. Expansion waves reflect from the jet boundary as weak compression waves and form an oblique shock. Behind the oblique shock, the flow is supersonic as well, but its Mach number is less than in the jet core.

In the core, the flow is isentropic, and ideal gas equations are correct for it. In the low-temperature media of the expanding gas condensation starts and clusters can exist. Then, passing through the normal shock, which is called Mach disc, entropy increases: the gas gets warm and clusters are likely to dissociate. To prevent this dissociation, a skimmer is used. It cuts the Mach disk, penetrates into the core of the jet and evacuates clusters before they collapse. The skimmer should be distant enough from the nozzle in order to let the clusters grow. On the other hand, it should not disturb the shock bottle structure. So, knowing the form and the structure of the flow is essential for optimizing cluster ion sources.

The picture given attributes to a jet from a sonic nozzle, i.e. a nozzle with only a converging part. However, a supersonic nozzle consisting of converging and diverging parts is usually used to generate GCIB [1,3]. Unfortunately, for such a nozzle we could not find any information on a jet structure under extensive clusterization. Typical ways of observing gas flows are rather complicated techniques such as schlieren-photography, electron-excited luminescence or Raman scattering [6–8]. Besides, these techniques demand additional equipment and substantial changes of the

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cluster formation chamber of a GCIB accelerator. Recently suggested technique utilizing dielectric barrier discharge [9] was not able to reveal the structure of the jet [10].

In this work, we suggest a simple technique of visualization of a jet by using glow discharge. It is suitable for using under pressure rates existing in GCIB accelerators, has very low requirements on the equipment and makes it possible to see the jet structure with a naked eye. Results of both experimental investigations and computer simulations of a supersonic jet are presented.

2. Experiment

The experiments were carried out using GCIB accelerator of Moscow State University [3]. The accelerator operates in pulsed mode. It means that the working gas is supplied through a pulsed valve installed before the nozzle. The pulse length was selected to be long enough for taking a photo.

The upper cover of the cluster formation chamber was made transparent. The skimmer was removed to provide more space for the experiments. Two configurations of electrodes were used to initiate glow discharge: an annular electrode and plane electrodes. Both configurations are shown in Fig. 2.

The annular electrode made of tungsten wire was placed coaxially with the nozzle. It had a diameter of 54 mm. The ring was under DC voltage, while the nozzle was grounded as well as the chamber walls and acted as the second electrode.

The two plane copper electrodes could be used instead of the annular one. They were placed symmetrically with respect to the nozzle axis. The distance between them was 65 mm; the longitudinal dimension was 62 mm. One of the electrodes was under DC voltage; the other was grounded as well as the nozzle and the chamber walls.

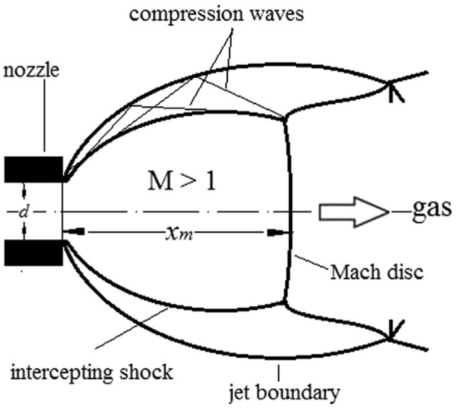

Fig. 1. Schematic view of a gas jet from a sonic nozzle.

In both cases, nozzle position relatively to the electrodes was set by motion of the nozzle holder.

To study the geometrical parameters of the jet depending on the inlet pressure and ambient pressure we used conical nozzles with critical cross-section diameters 140 μm and 400 μm. The length of diverging part and the half-opening angle were 20 mm and 6°, respectively.

Maximum pressure in the chamber was limited by the capability of the pumping system. In the operating mode of the accelerator, it does not exceed $8 \cdot 10^{-3}$ Torr. Depending on the duty factor of the pulsed valve and type of the working gas it can be raised up to $5 \cdot 10^{-2}$ Torr for a short time. Under such pressures, the glow discharge is initiated by the voltage of 0.3–2.5 kV depending on the experimental conditions.

For particular experimental conditions (working gas type and pressure, duty factor of the pulsed valve, configuration and position of the nozzle and electrodes) optimal values of the voltage and current exist to make a discharge snapshot. For example, excessive discharge current results in overexposed snapshot, and the jet structure is hardly distinguished. At the same time, insufficient current leads to low light intensity of the discharge.

Along with the experiments, computer simulations of a viscous gas flow in the axisymmetric nozzle and jet were performed. The flow was modeled by the system of two-dimensional unsteady Navier–Stokes–Fourier (NSF) equations. The system was written out in the divergence form and supplemented by the equations of state of an ideal gas and the boundary conditions on the boundaries of the computational domain. Terms describing convective transport in this system were approximated using a modified Godunov's scheme of high order of accuracy [11]. Terms describing diffusive (viscous) transfer were approximated using the finite volume method, which in the case of a uniform grid is reduced to a central difference approximation of derivatives. Advance in time was performed using the third order Runge–Kutta method. Influence of the gas condensation on the stream parameters was not taken into account on this stage.

Since the expansion ratio in the nozzle and jet is high (more than 1000), and at inlet temperature, the temperature at the nozzle exit falls below the critical value. Therefore temperature dependence of dynamic viscosity μ is described with the modified Satherland expression [12]:

$$\mu = \begin{cases} \mu(T_*)(T/T_*)^a, & T < T_* \\ \mu(T_*)(T/T_*)^{3/2}(T_*+S)/(T+S), & T \geq T_* \end{cases} \tag{1}$$

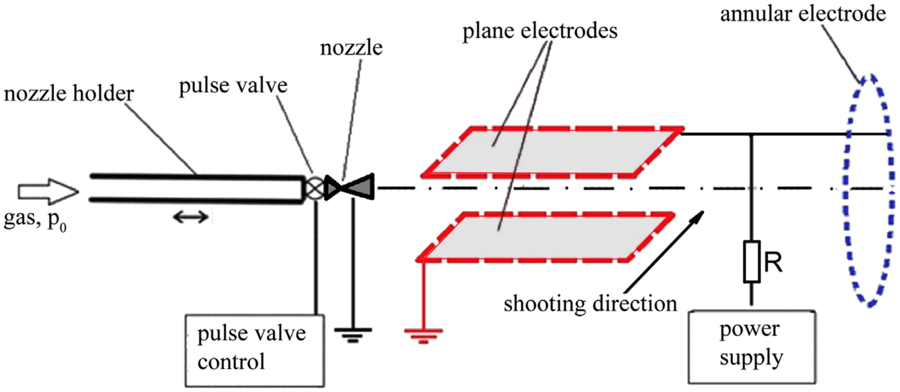

Fig. 2. Schematic diagram of flow visualization system using plane electrodes or an annular electrode.