Numerical simulation of high-intensity metal ion beam generation

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Abstract. The features and regularities of plasma-immersion formation of high-intensity repetitively pulsed beams of aluminum ions, as well as their transportation and ballistic focusing in an accelerating system with a curvilinear extracting potential grid electrode under application of negative bias with high pulse repetition rate of \( f = 10^5 \text{ Hz} \) are studied by numerical methods. It is shown that the amplitude and shape of the ion beam current pulse depend significantly on the dynamic conditions of space charge neutralization of the beam. In case of using of bias potential with high duty factor, e.g. conditions of limited time of vacuum-arc plasma preinjection, the process of transportation and ballistic focusing of the ion beam up to densities manifold exceeding the density of the preliminary injected plasma, it is possible to obtain conditions leading to the formation of a virtual anode. It is shown that secondary electrons can be one of the additional mechanisms of compensation of the beam space charge which results in the improvement of transportation of high-intensity beams of aluminum ions.

1. Introduction
In the conventional ion implantation methods pulsed, repetitively pulsed and continuous beams of metal and gas ions with energies ranging from 10 to 100 keV and average ion current densities of 1-100 \( \mu \text{A/cm}^2 \) are used [1-2]. The penetration depth of the alloying dopant at such processing modes does not exceed hundreds of nanometers.

High-intensity implantation at ion energies of several tens of keV and pulse current densities up to 5 mA/cm\(^2\) [3-6] showed the possibility of formation of intermetallic compounds at depths of several micrometers.

In terms of deep modification of materials, methods of high-current implantation of gas ions by ion beams with a current density of several mA/cm\(^2\) at low ion energies are of considerable interest [7-9] as well as high-intensity implantation of metal and mixed metal-gaseous ions.

Recently, a new approach to the formation of metal and gaseous ion beams, with a current density reaching tens and hundreds of mA/cm\(^2\) was described in Ref. [10-12]. It is shown experimentally that such ion current densities provide the possibility of doping materials with ions of gases and metals at depths of tens and hundreds of micrometers [13, 14]. The proposed method for the formation of low energy ion beams with a very high density is based on the combination of plasma-immersion extraction of ions and their subsequent ballistic focusing in the equipotential drift space of the potential electrode with the purification of beam from vacuum arc macroparticles due to the "solar eclipse" effect [10]. The formation of high-intensity ion beams is determined by the conditions of dynamic compensation of the
focused beam space charge in the drift space pre-filled by the injected plasma. Application of the numerical simulation method in addition to experimental studies greatly facilitates the task of understanding the complex physical processes of formation of pulsed and repetitively pulsed ion beams of metal, gases and semiconductors with ion energy in range of units of keV, at current densities reaching A/cm².

This work is devoted to the theoretical model of formation, transportation and ballistic focusing of high-intensity beams under the conditions of pre-injection of vacuum-arc plasma into the drift space.

2. Methods and numerical simulation results
The plasma and the ion beam were simulated by the number of particles of the order of 10⁵. The problem of transport and ballistic focusing of the ion beam in the equipotential space filled with plasma was solved using axially symmetric R-Z geometry (PIC code KARAT [15]). The processes of formation of the sheath and ion emission from the plasma boundary were not considered.

In the numerical model, it was assumed that the beam ions with an energy corresponding to the bias voltage $U$ are injected from the electrode (E), made in the form of a hemisphere with radius of $R=7.5$ cm, with a current of 1 A and transported to the collector (C) under ballistic focusing conditions. The initial plasma parameters are: the Maxwellian electron energy distribution function, the temperature of the plasma electrons is $T_e=10$ eV and the temperature of plasma ions is $T_i=1$ eV, secondary emission constant is 0.5, the directed plasma velocity along the symmetry axis is $v_{pl} \sim 2.7 \cdot 10^6$ cm/s [16]. The beam transport space is equipotential and is limited by the walls absorbing the charge. In the model, the depth of filling the beam transport region with the plasma (with density $n_{pl}$) was determined by the time of preliminary injection of the plasma, the average value of the density $n$ was determined over the entire volume of the drift space.

Figures 1-7 demonstrate the results of calculations for $U=-3$ kV, plasma and ion beam density at the entrance to the transport space $n_{pl}=2 \cdot 10^{10}$ cm⁻³ and $n_b=1.6 \cdot 10^9$ cm⁻³, respectively, are presented. In the spherical geometry, the density of fully neutralized ion beam is increasing as $r^2$ with the distance from the grid electrode to the current collector plate. Thus, the focusing of ion beam is accompanied with the formation of inhomogeneous potential well, which defines the movement of charged particles of plasma (ions and electrons). The calculations show, the lower the plasma density, the greater the time of the emission of plasma ions, and a correspondingly longer time to form the beam and the less current, that is observed in experiment [13, 14].

![Figure 1](image1.png)  
**Figure 1.** Calculated region geometry and the beam configuration portrait; E – grid electrode, C – collector, Sc – screen; $n=1.6 \cdot 10^{10}$ cm⁻³, $\tau=4$ μs.

![Figure 2](image2.png)  
**Figure 2.** Dynamics of the plasma electrons (g) and ions (r), beam ions (b) and secondary electrons (c) in the beam drift space; $\tau=4$ μs, $n=1.6 \cdot 10^{10}$ cm⁻³.
Figure 1 shows the calculation region geometry and the configuration portrait of the beam, arrow is velocity vector of the beam ions. Numerical studies have shown that the shading electrode (Sc) with a diameter of 4 cm on the grid electrode (E), which is necessary to prevent the deposition of vacuum arc macroparticles in the region of the ion beam focus on the collector, does not significantly reduce the density of the plasma and ion beam in the system (figure 1).

At the pulse duration of the bias potential of $\tau = 4 \mu s$, the time of preliminary plasma injection is 6 $\mu s$. Figure 2 shows the time dynamics of the number of charged particles in the drift space for the average plasma density of $n = 1.6 \cdot 10^{10}$ cm$^{-3}$ and the bias pulse duration $\tau = 4 \mu s$.

Figure 3 demonstrates the distribution of the longitudinal and radial components of the ion current density along the axis of the high-intensity beam of aluminum ion transportation corresponding to the above described conditions. Numerical calculations show that the radius of the beam on the collector does not exceed 1.5 cm when the target is located in the focus of the system.

**Figure 3.** Longitudinal (a) and radial components (b) of the total current density; $n = 1.6 \cdot 10^{10}$ cm$^{-3}$.

**Figure 4.** Trajectories of some ions of the beam (a) and kinetic energy of the corresponding ions (b).
The trajectories of some ions of the beam and the change of their kinetic energy at the time of 3 μs at the bias pulse duration of τ=6 μs are shown in figure 4. It is evident that the beam ions are transported in an inhomogeneous potential field, and the beam ions reaching the collector have a significant energy spread.

When the pulse duration of the bias potential is τ=8 μs, the time of preliminary injection of plasma is dramatically reduced and is equal to only 2 μs, and the average plasma density corresponds to just $n=8\times10^9$ cm$^{-3}$. Figure 5 shows the configuration portrait of the beam ions in this conditions at time $t=6$ μs. The deficit of plasma electrons and partial neutralization of the beam space charge leads to a significant potential drop, up to the formation of a virtual anode. However, in the process of ion beam transportation, the dynamic conditions of neutralization of its space charge may change. In the potential well, along with plasma electrons, secondary electrons from the surface of the target as a result of ion-electron emission are also captured, as well as accumulated in the process of ionization of the residual gas in the working chamber, gradually increasing the compensation of beam space charge. This process increases the current to the collector, due to a decrease in the current of the beam ions reflected from the virtual anode.

![Figure 5](image1.png)

**Figure 5.** Configuration portrait of an ion beam; E – grid electrode, C – collector, Sc – screen; τ=8 μs, $n=8\times10^9$ cm$^{-3}$.

![Figure 6](image2.png)

**Figure 6.** The currents of charged particles to the extracting grid electrode: r and c – plasma and secondary electrons, b – beam ions; τ=8 μs.

The current to the emission electrode has an oscillatory character (figure 6). This fact indicates the presence of the beam ion current reflected from the minimum of the potential well (virtual anode) and the non-stationary location of the virtual anode. Figure 6 also displays the currents of plasma ions and secondary electrons.

![Figure 7](image3.png)

**Figure 7.** The total current to the collector at different bias pulse durations; r and c – plasma and secondary electrons, b – beam ions.


Figure 7 shows the current pulses to the collector when the bias pulse duration is $\tau = 2, 4, 6$ and 8 $\mu$s. The first maximum on the curves is associated with the ion beam focusing; its amplitude depends on the density of the plasma particles and the steepness of the beam current edge.

Gradual increase of the ion current amplitude at $\tau = 8 \mu$s indicates an additional mechanism of compensation of the beam spatial charge over time. One of the mechanisms, as shown by calculations, can be ion-electron emission from the target surface.

When the displacement pulse duration $\tau = 8 \mu$s, the beam is transported under the conditions of virtual anode formation (figure 5), limiting the ion current to the collector. The part of the reflected ions from the potential well minimum falls on the grid, increasing its current. The other part passes into the sheath, reducing the current density in the ion layer, which leads to fluctuations in the emission plasma boundary and beam current. Frequency of oscillations of the location of the virtual anode depends on the current density of the beam, similar to the oscillations of the virtual cathode in vircator [17]. The experimentally observed intensive heating of the grid electrode up to melting at pulse duration $\tau = 8 \mu$s indicates the formation of a virtual anode with the reflection of a significant part of the beam ions from the positive potential barrier in the drift space and their oscillation relative to the grid anode.

3. Conclusion
The main processes accompanying the formation of focused pulsed periodic beams of aluminum ions with a current density of up to hundreds of mA/cm$^2$ are considered by numerical simulation methods. It is shown that at a pulse repetition rate of $10^5$ pulses/s and a short time of pre-injection of the vacuum arc plasma into the beam drift space (less than 4 $\mu$s), the beam is formed under conditions of incomplete compensation of the beam space charge by plasma electrons, and at a duty cycle of 2 $\mu$s, the beam is transported under conditions of virtual anode formation.

One of the additional mechanisms of compensation of the beam space charge over time can be ion electron emission from the target surface and electron generation during the interaction of the beam ions with residual gas atoms. Dynamic processes of neutralization of the beam space charge significantly affect the formation of the focused ion beam and its transportation.

Comparison of previously obtained experimental data and numerical simulation data indicate a high degree of agreement between the developed model of formation, transportation and ballistic focusing of high-intensity beams of low-energy ions and the peculiarities observed in the experiments.

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