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Process of Compensation of the Space Charge of a Negative Ion Beam in a Gas

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Abstract—The process of compensation of the space charge of a negative ion beam propagating through a neutral gas is investigated numerically. A comparison of the results obtained with experimental data unambiguously proves that, at high gas pressures, when the beam space charge is overcompensated, the electric field within the beam is determined by Coulomb collisions of the beam ions with plasma electrons. At low pressures, when the space charge is undercompensated, the field within the beam is determined by the dynamic processes related to oscillations of the beam current.

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1. INTRODUCTION

Efficient transportation of a high-current ion beam requires that the space charge of the beam ions be substantially compensated for by electric charges of opposite sign. When the beam propagates through a neutral gas, these charges arise due to gas ionization by the beam ions. In the initial stage of this process, the "anticompensating" particles (i.e., those having the charge of the same sign as the beam ions) are expelled from the ionization region ($r < r_0$, where r_0 is the beam radius) by the radial electric field. In a steady (generally, quasisteady) state, transverse fluxes of particles having charges of both signs are established that counterbalance (on the average) the generation of plasma particles (electrons and ions) in the axial region of the beam. Such a balance is the most general feature of the beamplasma system. The space-charge distribution that is established in the beam channel depends on the generation rate of plasma particles (and, accordingly, on their averaged radial fluxes) and determines the main sought-for parameter—the radial potential drop $\Delta\phi$ within the beam.¹ This parameter is directly related to the mechanisms governing the radial transport of the plasma components because it is these mechanisms that determine the level to which the beam channel is filled with plasma in a steady state.

The specific features of transportation of positive and negative ion beams are related to the large difference in the masses of the electrons and ions produced by gas ionization. In a positive ion beam, both the beam charge and the charge of the positive ions formed by gas ionization are neutralized by light electrons. Therefore, in the absence of a magnetic field, the beam space charge is always undercompensated. In the case of a negative ion beam, when heavy positive ions act as neutralizing charge particles, two regimes characterized by different mechanisms for generating radial chargedparticle fluxes (and, consequently, by very different compensation parameter $\Delta \varphi$) can be established. Depending on the gas pressure P, the beam can be either undercompensated ($\Delta \phi < 0$, $P < P_{cr}$) or overcompensated ($\Delta \phi > 0$, $P > P_{cr}$). In the former case, the radial electric field leads to the expansion of the propagating beam, while in the latter case, it results in the beam focusing, which came to be called "gas focusing" by analogy with a similar effect in electron beams. Studies of the plasma processes governing the value of $\Delta \phi$ in these two regimes are of fundamental importance for optimizing beam transportation.

At low gas pressures, the decompensation of a negative ion beam is caused by ion oscillations in the plasma [1]. The produced electrons are efficiently expelled from the beam by the beam electric field, and their equilibrium density is much lower than the density of the positive ions. In this case, the system may became unstable against the fundamental mode of ion oscillations with the half-wavelength on the order of the beam diameter.² The onset of such oscillations prevents the beam channel from being filled by positive ions, because, at a given generation rate, the density of these particles within the beam is low due to the anomalously high average velocity with which they are removed from the beam. As a result, the beam remains substantially unneutralized [1, 2], $\Delta \phi < 0$. Another decompensation factor is beam-current oscillations caused by plasma instabilities in the ion source itself [1, 2]. If the

¹ The average electric field in the beam is $E_r \propto \Delta \varphi = \varphi(r=0) - \varphi(r=r_0)$.

² When the Debye length is larger than the beam radius, such oscillations cannot be screened by the plasma electrons.

onset of ion oscillations were excluded, the value of $\Delta \phi$ would be appreciably higher, remaining nevertheless negative. In this case, the radial drift of positive ions would be determined only by Coulomb collisions with the beam ions.

At pressures higher than the critical pressure P_{cr} , the electron density is considerably higher and the beam's steady state is characterized by the following features.

(i) The influence of electron and ion oscillations on the formation of the space charge distribution is insignificant [1] because, in particular, the wavelengths of the excited ion oscillations are short due to an increase in the screening effect of the plasma electrons.

(ii) Due to intense generation of positive ions (the heavy, low-mobility plasma component), their quasisteady distribution corresponds to a positive beam potential, $\Delta \phi > 0$; i.e., the beam space charge is overcompensated and the radial flux of the positive ions is mainly caused by the electric field.

In the beam channel, there are also slow electrons that cannot overcome the potential barrier of height $e\varphi(r=0)$, as is the case with a positive ion beam.³ The established radial flux of slow electrons is determined by their heating in Coulomb collisions with the beam ions [1, 2]. At high gas pressures, the beam's steady state can be analyzed by using a simplified physical model in which plasma instabilities are discarded.

The potential drop $\Delta \varphi$ can be calculated from the energy balance equation that takes into account the energy contribution from the beam ions and the losses caused the drift of plasma particles toward the wall. Of course, this equation will be approximate because some parameters are unknown and may be determined only by solving the problem self-consistently. For example, in order to correctly write the energy balance equation, it is necessary to predetermine not only the plasma component responsible for the main energy losses from the beam channel but also the group of particles within this component that mostly contribute to these losses. Previous investigations performed by different authors have shown that models based on qualitative considerations can yield contradictory results.

In [1, 2], the average focusing field (the value of $\Delta \varphi$) in the regime with $P > P_{cr}$ was determined from the energy balance equation that took into account the heating of the compensating electrons in Coulomb collisions with the beam ions. The electrons that acquire the energy sufficient to overcome the potential barrier leave the beam channel (their velocity at the beam periphery is close to zero). Note that, in this case, their kinetic energy transforms into the potential energy of the electric field. The energy is carried away by positive ions. The estimated values of $\Delta \phi$ agree well with experimental data.

In [3, 4] (as well as in [1, 2]), the degree to which the ion beam was compensated was determined from the energy balance equation for electrons with allowance for Coulomb collisions between electrons and the beam ions. However, the energy balance was written for all the beam–plasma system rather than for the compensating electrons. Accordingly, energy losses due to the escape of positive plasma ions were not taken into account and the contribution from electrons to energy losses was highly overestimated.

Taking into account that the problem under study concerns the basic issues of the ion-beam physics, we performed mathematical simulations of the beam dynamics up to the steady stage by using a more general model based on the particle-in-cells (PIC) method for an axisymmetric system. The results obtained show that the approach developed in [1, 2] adequately describes actual processes. At high pressures, the dependences of the electric field on the beam and gas parameters agree with experimental data and estimates obtained in [1, 2]. It is shown that, when Coulomb collisions are discarded, the electric field within the beam tends asymptotically to zero with time; this result confirms the idea of the defining role of these collisions in the formation of the steady focusing field within the beam.

2. QUALITATIVE CONSIDERATIONS

As was mentioned above, the main reason why space-charge neutralization in negative ion beams differs qualitatively from that in positive ion beams is the large mass of compensating particles (positive ions). It is due to this circumstance that the space charge of a negative ion beam can be overcompensated at high gas pressures. The critical gas pressure at which $\Delta \phi = 0$ can be estimated from the set of balance equations for plasma electrons and ions and the quasineutrality condition:

$$n_{-} \nabla_{-} n_{a, cr} \sigma_{i} \pi r_{0}^{2} = n_{i} \nabla_{i} 2 \pi r_{0},$$

$$n_{-} \nabla_{-} n_{a, cr} \sigma_{e} \pi r_{0}^{2} = n_{e} \nabla_{e} 2 \pi r_{0},$$

$$n_{-} + n_{e} = n_{i}.$$
(1)

Here, n_{-} , n_i , n_e , and n_a are the densities of the beam ions, plasma ions, electrons, and neutral gas particles (molecules or atoms), respectively; σ_i and σ_e are the cross sections for the production of positive ions and electrons (with allowance for gas ionization and charge exchange of the beam ions; in this case, $\sigma_e > \sigma_i$); v_i and v_e are the average transverse velocities of plasma ions and electrons produced in collisions of the beam ions with neutral gas particles; v_- is the average transverse velocity of the beam ions; and r_0 is the beam radius. Since $v_e \ge v_i$ and the charge-exchange rate at the critical pressure is relatively low, the value of $n_{a, cr}$ can be

³ This fraction of the plasma electron component will be referred to as compensating. Note that, in this case, we speak of the compensation of the positive ion charge rather than the neutralization of the negative ion beam. The faster electrons escape to the chamber wall of radius *R* and along the beam propagation direction. The wall potential is assumed to be $\varphi(r = R) = 0$.

estimated by assuming that $n_e \ll n_i$ or $n_- \approx n_i$ in the first equation of set (1). Then, for the critical density of neutral particles, we have

$$n_{a, cr} = \frac{2v_i}{v_- r_0 \sigma_i \left(1 - \frac{v_i \sigma_e}{v_e \sigma_i}\right)} \approx \frac{2v_i}{v_- r_0 \sigma_i}.$$
 (2)

When the pressure is lower than the critical one ($\Delta \phi < 0$), all the produced electrons freely escape from the

beam and their density is $n_e \sim n_- \frac{V_i}{V_e} \ll n_-$. In this case, the difference between n_i and n_- is insignificant, i.e., the system may be considered two-component. At pressures higher than the critical one, the electric field confines slow electrons within the beam; therefore, the system becomes a three-component one, as is the case with a positive ion beam. Note that the electron density increases with gas pressure more rapidly than the density of positive ions. Let us estimate the value of $\Delta \varphi$ for regimes in which $P > P_{\rm cr}$.

In [5], the radial potential drop within the beam in this regime was determined from the balance equation for electrons,

$$n_{-} \nabla_{-} n_{a} \sigma_{e} \pi r_{0}^{2} = n_{e} \nabla_{e} e^{-\frac{e \Delta \varphi}{kT_{e}}} \times 2\pi r_{0}, \qquad (3)$$

where T_e is the electron temperature. It follows from Eq. (3) that $e\Delta\phi$ is approximately equal to a few units of kT_e . This estimate is certainly correct because it is based on the only assumption that the compensating electrons are distributed within the beam according to the Boltzmann law, which is usually satisfied with a good accuracy because the characteristic electron-electron collision time is considerably shorter than the lifetime of the compensating electrons. It is evident, however, that expression (3) is not a solution to the problem because the parameter kT_e (as well as $\Delta \varphi$) is unknown. In [6], the energy balance equation was used to find the dependence of $\Delta \varphi$ (and, consequently, kT_{e}) on the beam and gas parameters. The compensating electrons are slow electrons whose kinetic energy ε_{k0} at the instant of their formation is too low for they can escape from the potential well of the beam. It is these electrons that are confined by the beam and determine the corresponding space charge. The contribution from fast electrons with initial energies $\varepsilon_{k0} > e\varphi(r)$ (where *r* is the coordinate of an electron at the instant of its formation) is insignificant because they very rapidly leave the beam.

Continuous ionization of the gas in the beam channel implies that there are physical mechanisms that provide equilibrium between the generation of compensating electrons and their escape from the beam though their energy is lower than the threshold value: $\varepsilon_{k0} < e\phi(r)$. Such mechanisms are related to the heating of slow electrons by the beam ions. The energy can be transferred due to both Coulomb collisions and collective processes. In order to estimate the minimum electric field in the beam, it is sufficient to consider only Coulomb collisions. In this case, the compensating electrons gradually acquire energy in electron–ion interactions occurring within a Debye sphere, in contrast to, e.g., neutral molecules, whose energy can change abruptly under the action of short-range forces arising in their collisions with other molecules. As soon as the kinetic energy of electrons reaches the level equal to the height of the potential barrier, they leave the beam channel, their final velocity being infinitesimally low.⁴ Based on these consideration, we can write the following equation for the energy balance of the compensating electrons [1, 6]:

$$\int_{0}^{r_{0}} 2\pi r dr \int_{0}^{e\phi} (e\phi - \varepsilon) f(\varepsilon) d\varepsilon = \alpha \frac{n_{-}n_{e}}{v_{-}} \frac{e^{4}\pi r_{0}^{2}}{m_{e}}, \qquad (4)$$

where $\alpha = 4\pi \ln \left[\frac{v_{-}^{3}}{n_{e}^{1/2}} \frac{m_{e}^{3/2}}{1.78\pi^{1/2}e^{3}} \right], f(\varepsilon)$ is the energy dis-

tribution function of the electrons produced in collisions of the beam ions with neutral particles.

The left-hand side of Eq. (4) is the power that should be transferred to trapped electrons per unit length of the beam channel to provide their escape from the beam, while the right-hand side is the power transferred to these electrons due to Coulomb collisions with the beam ions. Assuming for simplicity that

$$\varphi = \Delta \varphi (1 - r^2 / r_0^2), \quad f(\varepsilon) = e \varphi_i / (\varepsilon + e \varphi_i)^2 \quad (4a)$$

(where φ_i is the energy of gas ionization), we obtain the following expression for $\Delta \varphi$:

$$\Delta \varphi = \sqrt{3\alpha} \left(\frac{M}{m}\right)^{1/2} \left(\frac{1}{n_a \sigma_i}\right)^{1/2} \left(\frac{\varphi_i}{U_0}\right)^{1/2} e n_{-}^{1/2} \left(1 - \frac{n_{a, \text{cr}}}{n_a}\right)^{1/2}.$$
 (5)

Here, the voltage U_0 determines the energy of the beam ions, eU_0 , and M is the mass of an ion.

It can be seen from expression (5) that the radial potential drop within the beam is determined by the beam and gas parameters; therefore, this expression is a solution to the problem. Taking into account Eq. (3), it is easy to calculate the temperature of the compensating electrons in terms of the beam parameters. Note that, in the absence of Coulomb collisions (formally, at $\alpha = 0$ in Eq. (4)), the radial potential drop would be zero. This result can be easily interpreted: without an external energy source that heats the compensating electrons, the beam channel would be finally filled with electrons with initial energies $\varepsilon_{k0} \approx 0$ to a level corresponding to the total compensation of the space charge in the system.

⁴ It should be noted that, when the trapped electrons overcome the potential barrier, they do not carry away energy from the beam channel. Their kinetic energy transforms into the energy of the electric field and is then transferred to the positive plasma ions that are expelled from the beam.



Fig. 1. Electric potential at the beam axis, $\varphi(r = 0)$ (curve *I*), and radial potential drop within the beam, $\Delta \varphi$ (curve *2*), as functions of the gas pressure: (a) $P < 2 \times 10^{-4}$ Torr and (b) $P > 2 \times 10^{-4}$ Torr.

It should also be noted that, in [6], the value of $\Delta \phi$ in a positive ion beam was found in a similar way. Moreover, above estimates agree well with experimental data in both cases. As for the results of [3, 4], whose drawbacks were pointed out in the Introduction, the energy balance equation written in those papers would lead to expression (4) if this equation were corrected to take into account both the dominant role of slow electrons in the formation of the space charge and the removal of energy from the beam by positive plasma ions.

3. COMPUTATIONAL SCHEME

The computational model was based on the PIC method. It was assumed that a homogeneous ion beam with the radius $r_0 = 2.5$ cm, energy $eU_0 = 15$ keV, and current $I_{-} = 5$ mA propagated along the axis of a cylindrical chamber (with a diameter of R = 7.5 cm and length of L = 50 cm) filled with argon. The argon pressure was varied within the range 10^{-5} – 1.3×10^{-3} Torr. The system was assumed to be axisymmetric and axially homogeneous. The boundary conditions for the electric potential were $\varphi(r = R) = \frac{\partial \varphi}{\partial r}\Big|_{r=0} = 0$. In

solving the equations of motion for charged particles (with a time step Δt), the magnetic field of the beam was ignored. After every time step Δt , additional charged particles were added to each computational cell ΔV_k in accordance with the generation rates of ions, $G_i = n_V n_a \sigma_i \Delta V_k$, and electrons, $G_e = n_V n_a \sigma_e \Delta V_k$, where $\sigma_i = 3.5 \times 10^{-16} \text{ cm}^2$ and $\sigma_e = 2.5 \times 10^{-15} \text{ cm}^2$ (taking into account the neutralization of plasma ions in the reaction $H^- + Ar \longrightarrow H + Ar + e$ [7]. The initial coordinates of the produced particles within a cell were chosen randomly (with an even probability distribution). The energy distribution function of the positive ions produced by gas ionization was chosen to have the shape of a step with the cutoff energy 0.6 eV. Simulations performed with other shapes of this function yielded almost the same results. The electron energy distribution function was taken in form (4a), multiplied by a normalizing factor.

Coulomb interactions of the beam ions with positive plasma ions were taken into account by introducing a correction to the momentum of each particle at every time step. These corrections were calculated in accordance with energy losses of a beam propagating through an electron (ion) gas.

In order to find the potential $\varphi(r)$ from Poisson's equation, the distributions of the charge densities of the system components were determined by the cloud-incell method. After the electric field $E_r(r)$ was calculated, the computational procedure (including the solution of the equations of motion, generation of new particles, correction of the particle momenta, and solution of Poisson's equation) was repeated again at a new time step until the electric potential reached a steady distribution [8, 9].

4. RESULTS OF NUMERICAL SIMULATIONS

Figure 1 shows the calculated dependences of the electric potential at the beam axis (curve *I*) and the potential drop between the axis of the beam and its boundary, $\Delta \varphi = \varphi(r=0) - \varphi(r=r_0)$ (curve 2), on the gas pressure. At a pressure of $P = 1.65 \times 10^{-5}$ Torr, both of these quantities vanish (Fig. 1a). Thus, the critical pressure obtained in these simulations is close to the estimate $P_{cr} \approx 1.82 \times 10^{-5}$ Torr, calculated from formula (2). Note that, at low pressures, when the beam potential is negative, the computational model, which assumes that the system is homogeneous along the *z* axis and disregards effects related to the modulation of the beam current due to plasma oscillations in the ion beam [1, 2], yields too low values of $|\varphi(r=0)|$.

Let us consider the regime of high pressures in more detail. Figure 2 shows the radial distribution of the potential in a steady state at a pressure of $P = 1.5 \times 10^{-3}$ Torr. The beam is seen to be substantially over-compensated by positive ions. This indicates that electron heating is so efficient that the electrons intensely



Fig. 2. Radial profile of the potential in the system at a gas pressure of 1.3×10^{-3} Torr.

escape from the chamber volume. When Coulomb collisions between electrons and the beam ions are ignored, the potential at the beam axis, $\varphi(r = 0, t)$, tends asymptotically to zero as time elapses.

Let us consider the electron energy distribution function (see Fig. 3). The electrons with energies higher than the potential barrier $\Delta \varepsilon \approx 10.7 \text{ eV}$ (Fig. 2) very rapidly escape to the chamber wall. Therefore, $f(\varepsilon) \approx 0$ at $\varepsilon > \Delta \varepsilon$. We emphasize that the above features of the system of particles trapped by the electric field and forming the space charge are very important for correctly deriving the energy balance equations. When $P > P_{cr}$, the energy is carried away only by the electrons with the maximum (on the trajectory) kinetic energy ε_{max} exceeding the threshold value $\Delta \varepsilon$. However, the number



Fig. 3. Electron energy distribution function at a gas pressure of 1.3×10^{-3} Torr.

of such electrons is very small: as soon as ε_{max} exceeds $\Delta \varepsilon$, the electron rapidly leaves the beam channel and carries away the energy $\varepsilon_{max} - \Delta \varepsilon$; in this case, $(\varepsilon_{max} - \Delta \varepsilon)/\varepsilon_{max} \ll 1$. Most of the energy transforms into the energy of the electric field of the beam. Assuming that the electron distribution at high energies is Maxwellian (without a cutoff at $\varepsilon > \Delta \varepsilon$), the authors of [3, 4] substantially overestimated the energy carried away from the system by the electrons. Actually, the beam energy is mainly carried away by positive ions, which acquire energy from the electric field.

The data presented in Fig. 4, which shows the electric potential at the beam axis (curve *I*) and the potential difference $\Delta \varphi$ (curve *2*) as functions of the beam current density, confirm the correctness of estimate (5): both values are seen to be nearly proportional to $\sqrt{j_-} \sim n_-^{1/2}$.

Finally, let us compare the results of numerical simulations with the dependences observed experimentally in [1, 2]. The experiments were performed with a steady 20-keV H⁻ beam at currents of up to 6 mA. Figure 5 shows the dependences $\varphi(r = 0, P)$ for different gases. It can be seen that, in accordance with expression (2), the critical gas pressure $P_{cr} \sim v_i$ decreases with increasing molecular mass (which is related to a decrease in the average radial velocity of molecules). The values of the beam potential in the range of high pressures are close to those obtained in numerical simulations. In order to more thoroughly compare experimental and calculated data (including estimates by formula (4)) in the range of high pressures, Fig. 6 presents the radial potential drop as a function of the beam current density. A comparison of Figs. 4 and 6 shows that the simulation results agree well with both the experimental data and the estimates based on the energy balance equation for the compensating electrons. As for the regime of low pressures, it can be seen from Fig. 5



Fig. 4. Electric potential at the beam axis, $\varphi(r = 0)$ (curve *1*), and radial potential drop $\Delta \varphi$ (curve *2*) as functions of the beam current density at a gas pressure of 5.0×10^{-4} Torr.

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Fig. 5. Measured dependences of the potential at the beam axis on the gas pressure for (1) krypton, (2) air, and (3) helium at $I_{-} = 4$ mA and $eU_{0} = 10$ keV.



Fig. 6. Calculated radial potential drop $\Delta \varphi$ as a function of the beam current density for (1) air and (2) krypton. The circles show the experimental data for krypton.

that the absolute values of the negative beam potential considerably exceed those calculated with allowance for Coulomb collisions (Fig. 1a). As was mentioned above, such a discrepancy is related to the influence of dynamic effects, which were not taken into account in our numerical simulations but are present in the experiment because of the beam current modulations caused by plasma oscillations in the ion source [1, 2]. Indeed, the frequency of current oscillations (200–500 kHz) considerably exceeds the reciprocal of the ionization time. Therefore, over a half-period of oscillations, when the current is higher than its mean value, the number of produced positive ions is insufficient for the compensation of the beam space charge. Accordingly, the alternating component of the space charge is compensated incompletely; i.e., there are oscillations of the where I_{-} is the alternating component of the beam current and α is the modulation depth. Since the modulation depth of the beam current reaches 0.2, the amplitude of the alternating component of the electric potentials can amount to a few volts, which agrees with the data from a thermoprobe (Figs. 5, 6).

5. CONCLUSIONS

A comparison of the numerical results with the experimental data, as well as with the estimates obtained from the energy balance for the compensating electrons, allows us to draw the following conclusions.

(i) The electric field within a negative ion beam propagating through a gas at an overcritical pressure (i.e., in the regime of gas focusing) is determined by Coulomb collisions between the beam ions and plasma electrons.

(ii) The electric field within a negative ion beam at an undercritical gas pressure (i.e., when the system is in fact two-component) is determined by the dynamic effects.

(iii) Estimates obtained in [1, 2] from the energy balance equation for the compensating electrons fairly correctly describe the electric field within a negative ion beam in the regime of gas focusing.

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