Ion Mean Charge State in a Biased Vacuum Arc Plasma Duct

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***Abstract*—Vacuum arc or cathodic arc metal plasma sources are attractive and convenient for depositing high-quality thin metal films and metallurgical coatings. It is a common practice to use a curved magnetic filter duct to eliminate macroparticle contamination and to bias the duct wall with a positive voltage to enhance the throughput of the metal plasma. The metal plasma usually consists of several charge states and time-of-flight (TOF) experiments show that the mean charge state of the metal ions decreases with increasing bias and magnetic field applied to the filter duct. We also derive the throughput of ions with different charge states at different bias voltage and magnetic field by the particle-in-cell (PIC) method. The ion trajectory is simulated neglecting the influence of electron charge. Our results show that the simulated mean charge state displays a similar decreasing trend as the bias voltage and magnetic field strength are increased. Phenomena such as reduction of the mean charge state at high magnetic field strength and bias can be explained in terms of standalone multiply charged metal ions under the influences of magnetic and electric forces inside the filter duct.**

***Index Terms*—Ion charge states, plasma duct, vacuum arc sources.**

I. INTRODUCTION

VACUUM arc or cathodic arc metal plasma sources are widely used in plasma-based applications especially for the fabrication of thin films and coatings [1]–[4]. The process can be carried out either at high vacuum or in a low-pressure gaseous environment, and films can be composed of metals, ceramics, diamond-like carbon, some semiconductors and superconductors, and other materials. The method is thus a versatile and powerful plasma tool for the synthesis of novel and technologically interesting surfaces. The contamination of the thin metal films by macroparticles, droplets of resolidified cathode debris of dimensions in the broad range from 0.1 to 10 μm, is the major disadvantage precluding a wide application of vacuum arc plasma sources in industry. Macroparticle contamination in general leads to imperfect films, and it is often important to remove this contamination with a macroparticle filter [4], [5]. A common filter consists of a curved solenoidal magnetic duct of field strength typically several hundred Gauss to perhaps 1 kG, and of angular extent (bend angle) typically 45–90 [6]–[9], [22], [23]. The metal plasma is transported through the bent duct, whereas the macroparticles collide with the duct wall due to inertia and are lost from the plasma stream. One drawback of the magnetic duct is its low plasma transport efficiency and the consequent reduction of the usable plasma flux. In order to increase the plasma throughput, the duct wall area is often positively biased, either *in toto* or by using an electrode facing the plasma on the outer quadrant of the duct inner surface by means of a Bilek bias plate [10], [11]. A Bilek plate is simply a conducting plate inserted inside the duct and covering a quarter or half of the inner surface of the duct at its outer radius. It is biased positively to a few tens of volts and serves as an alternative to biasing the duct itself.

For typical magnetic field strength, the electrons are magnetized but the ions are not. Electron motion inside the duct of the vacuum arc metal plasma source is thus an important phenomenon. The internal electric field inside the plasma will guide the ions through the filter duct, i.e., a plasma optics model is appropriate [6], [12]. The charge state distributions of metal ions in a vacuum arc plasma generally range from $+1$ to $+5$, with a mean charge state between $+2$ and $+3$, depending on the materials [13]. The mean ion charge state of several metal plasmas transported through a magnetic filter under the influence of different magnetic field strengths and bias voltage has been investigated [14]–[16]. Based on time-of-flight (TOF) data, the mean charge state increases at low magnetic field and then steadily decreases as the field is increased [16]. At high field, the mean charge state is significantly lower than the unfiltered value [16]. The total throughput of the metal ions or ion flux can be measured by placing a collector plate in front of the duct exit and applying -50 V to the collector plate to repel the electrons [14], [15]. As the bias voltage on the Bilek plate is increased, the current mea–sured on the collector plate goes up, attains a maximum value, and finally reaches a plateau.

In this paper, we present the results of our measurements of the mean charge state as determined by a TOF method, for a Ti plasma ions for different bias voltages with fixed magnetic field strength. The results show that the mean charge state decreases as the bias is increased. The ion flux increases at low voltage and exhibits a maximum. This result is similar to that of a collector plate current experiment [14], [15]. We subsequently simulate the ion trajectories and compute the throughput of standalone ions without any plasma electrons for different charge states at

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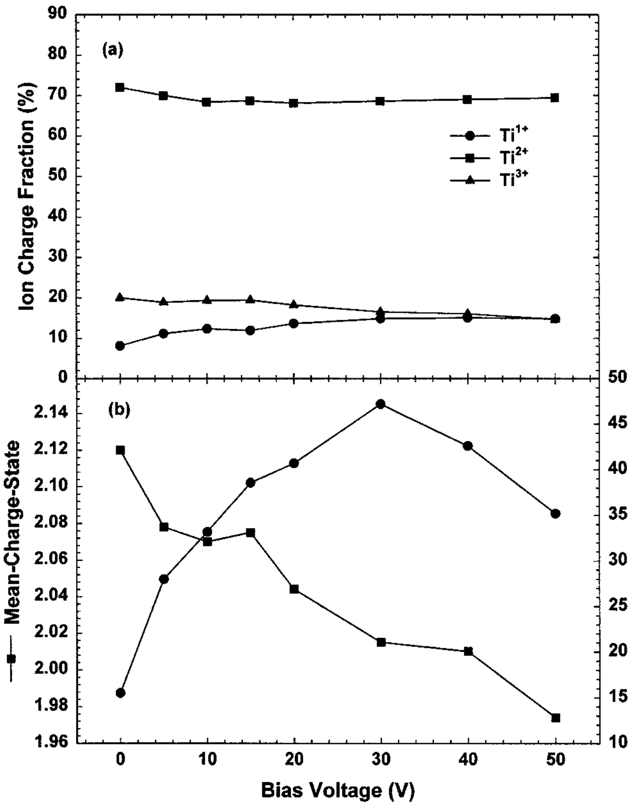


Fig. 1. Measured charge state fraction, throughput flux, and mean charge state of the transported Ti ion plasma as a function of the bias voltage.

different bias and magnetic field using a particle-in-cell (PIC) method. It is observed that the computed mean charge state displays the same tendency.

II. Experimental

The TOF mass spectrometer hardware and experimental conditions have been described elsewhere [17]. The TOF measurements were made at about 100 μs after arc ignition. The vacuum arc current pulse was rectangular, of amplitude about 200 A and duration about 250 μs. In these experiments, we used a 90° duct with a major radius of 10 cm and minor radius of 3.5 cm with a bias plate covering half the area of the outer duct wall. The magnetic filter duct was made from coiled copper wire secured with glass tape. The filtered Ti metal plasma enters the TOF setup and the ions are separated and detected according to their arrival time or mass-to-charge ratio. The plasma density within the duct is on the order of 10^{12} cm^{-3}. The vacuum arc metal plasma consists mainly of Ti^{+}, Ti^{2+}, and Ti^{3+}, and the charge state distribution, throughput ions, and mean charge state of the transported Ti ion plasma are shown in Fig. 1 as a function of the bias voltage. The duct magnetic field strength was 480 Gauss. Each data point represents an average of over 50 plasma pulses. It can be seen that the relative amount of Ti^{+} increases with increasing bias voltage. This indicates that at a higher bias, the transport efficiency is better for the singly charged Ti^{+} ions. The mean ion charge state continues to diminish as the bias voltage is increased. The combined throughout of the ions (total ion flux) reaches a maximum at 30 V.

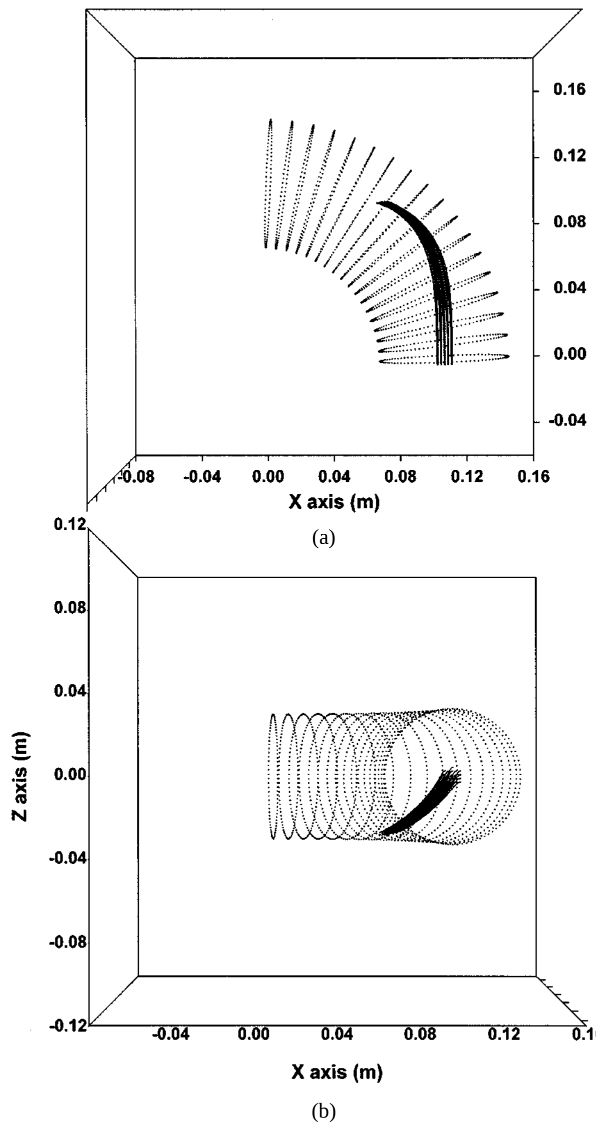


Fig. 2. Trajectories of the Ti^{+} ions at a magnetic field of 0.25 Telsa at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane. The potential of the duct wall and bias plate is equal to zero.

III. Theoretical Simulation

The three-dimensional (3-D) model used to simulate the ion trajectory along the duct filter in cylindrical coordinates (ρ, ϕ, z) has been described elsewhere [18]. The symmetry axis of the curved duct lies on the $z = 0$ plane and the center of the major curvature is placed at the origin. The magnetic field is generated by the coils surrounding the duct. The field $d\vec{B}$ at a point due to an element of the duct coil is represented by

$$d\vec{B} = \frac{\mu_o In\,(\rho d\phi)\; d\vec{l}\vec{r}}{4\pi r^3} \tag{1}$$

where

- μ_o permeability of free space;
- I current in the duct coils;
- n number of turns per unit length;
- $\rho d\phi$ length of the element along ϕ;
- $\vec{r}$ vector between the point and the element;
- $d\vec{l}$ vector tangent to the surface of the duct [18].

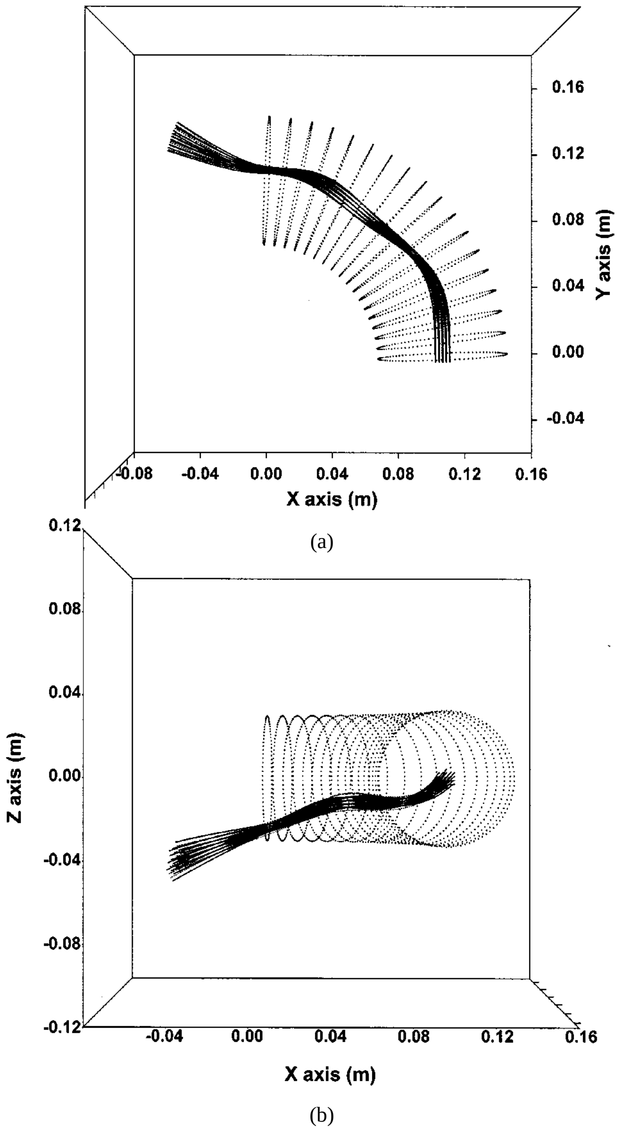


Fig. 3. Trajectories of the Ti^{+} ions at a magnetic field of 0.5 Telsa at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane. The potential of the duct wall and bias plate is equal to zero.

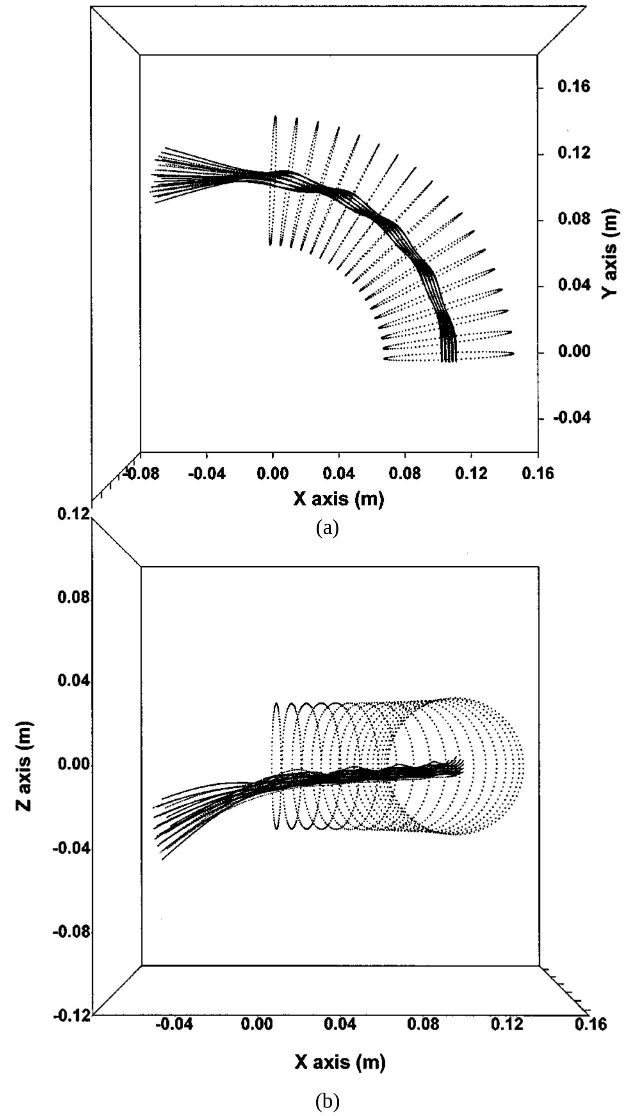


Fig. 4. Trajectories of the Ti^{3+} ions at a magnetic field of 0.5 Telsa at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane. The potential of the duct wall and bias plate is equal to zero.

The ultimate magnetic field at a point in space can be calculated by integrating (1) for all the duct coils.

An electric field is generated by the positive voltage applied to the bias plate placed at the outer wall of the curved duct. The potential Φ in space can be expressed by Poisson's equation

$$\nabla^2\Phi = -\frac{\left(\sum q_i n_i - q n_e\right)}{\varepsilon_o} \tag{2}$$

where

q elementary charge;

q_i constituent charge;

ε_o permittivity of free space;

n_i and n_e ion and electron densities, respectively.

The throughput and radial uniformity of plasma transported through the filter duct have been investigated and compared to estimates based on the duct magnetic field strength and shape [10], [11]. The trajectories of the ions passing through the filter duct have not been examined. In the work presented here, the main concern is the motion and trajectories of individual ions passing through the filter duct. The internal plasma field has been neglected by assuming n_i and n_e to be zero. In this way, the strength and effect of the external electric and magnetic field can be investigated in the simulation.

We did not use special torodial solenoid coordinates in this work [21]. This kind of special coordinate system is complex and difficult to differentiate, especially when an asymmetric field structure like the electric field created by a quarter-section Bilek bias plate is involved. The only disadvantage to using cylindrical coordinates is that the circular boundary of the duct wall will not lie on the rectangular mesh along the (r, z) plane [18]. This can be solved by simply adopting an "irregular physical boundaries" method to express the first and second order

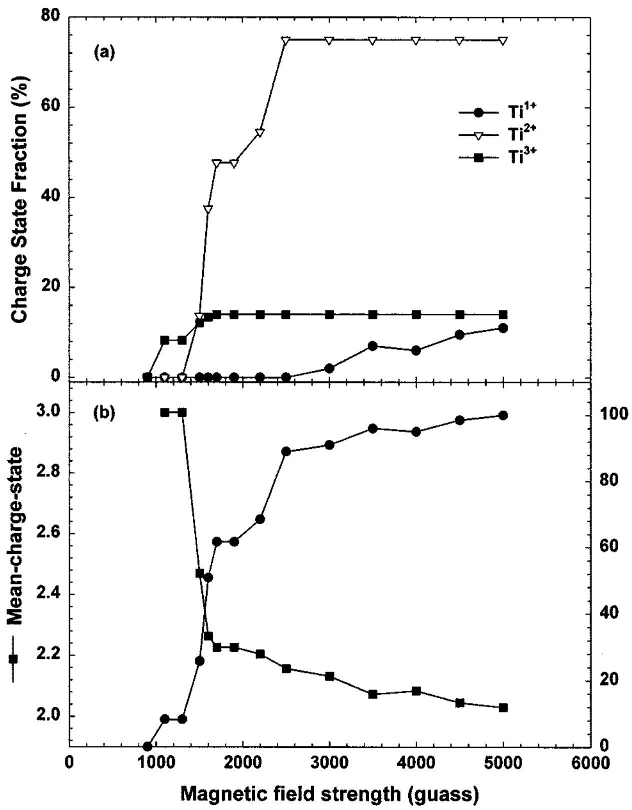


Fig. 5. Computed charge state fraction, throughput flux, and mean charge state of the transported Ti ion plasma as a function of the magnetic field strength.

derivatives in terms of the values at the boundary rather than the node [20]. In cylindrical coordinates, this becomes

$$\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial \Phi}{\partial \rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial \phi^2}+\frac{\partial^2\Phi}{\partial z^2}=0. \tag{3}$$

Equation (3) can be solved by the finite difference method [18]. The default potential of the duct wall is equal to zero. The Bilek bias plate covers a quarter of the duct wall at its outer radius. Therefore, the potential of the duct wall covered by the bias plate is equal to 30 V. The potential of each grid point is obtained by iteration. The trajectory of a charged particle under the influence of the electric $\vec{E}$ and magnetic $\vec{B}$ fields can be described by the kinematic equations

$$m\frac{d\vec{V}}{dt}=q\left(\vec{E}+\vec{V}\times\vec{B}\right) \tag{4}$$

$$\frac{d\vec{r}_p}{dt}=\vec{V} \tag{5}$$

where

q charge of the particle;
$\vec{V}$ velocity;
$\vec{r}_p$ position of the particle.

$\vec{E}$ and $\vec{B}$ are position dependent. The position of the ion is numerically updated using (5). The iterative process is repeated at the updated position until the end of the simulation. A total of 16 particles (ions) are evenly distributed at the beginning of the center of the filter duct within a circle of radius $= 0.5$ cm.

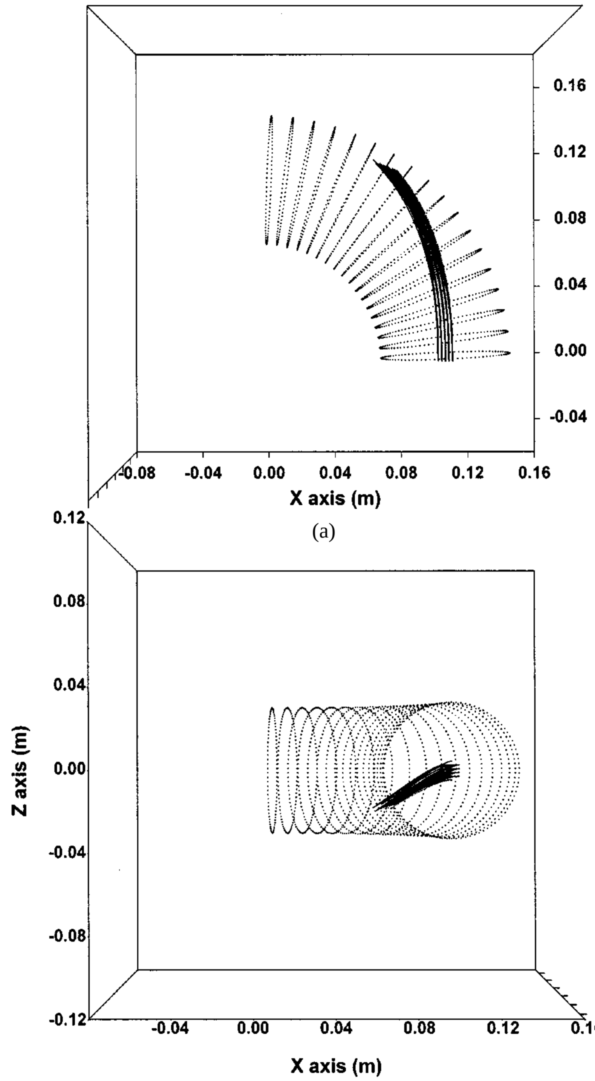


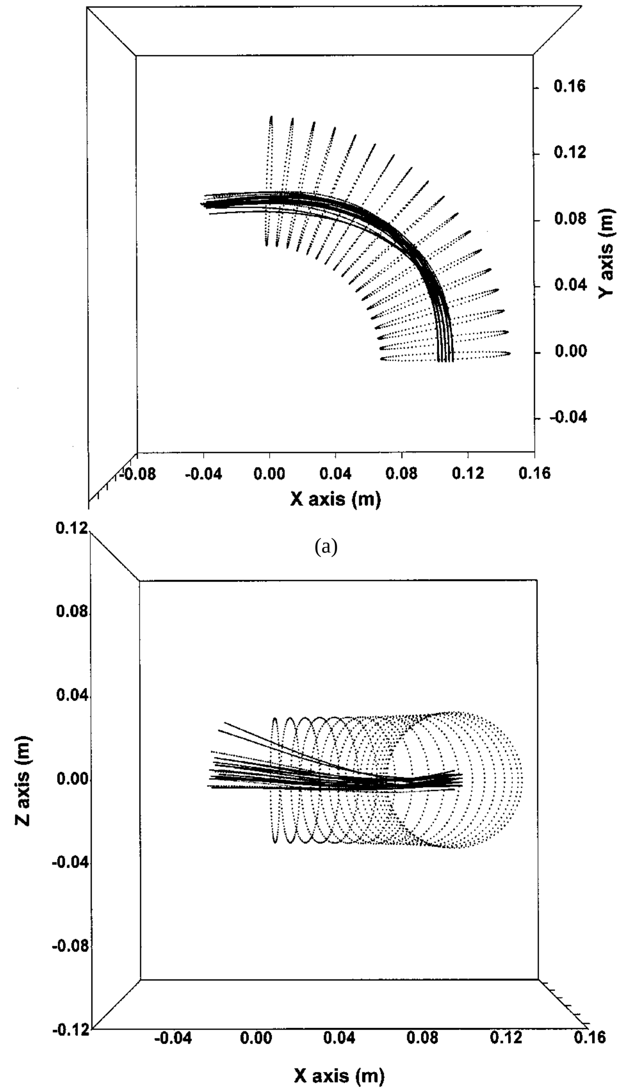
Fig. 6. Trajectories of the Ti^{2+} ions at 10 V bias voltage and 0.048 T magnetic field at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane.

The initial velocity of the ions is taken here to be 1.5×10^4 m/s normal to the duct entrance. Thus, we make the approximation that ions of different charge states have the same initial velocity. Ions at different starting positions will travel through the filter duct at different trajectories.

IV. Results

A. Magnetic Field Dependence

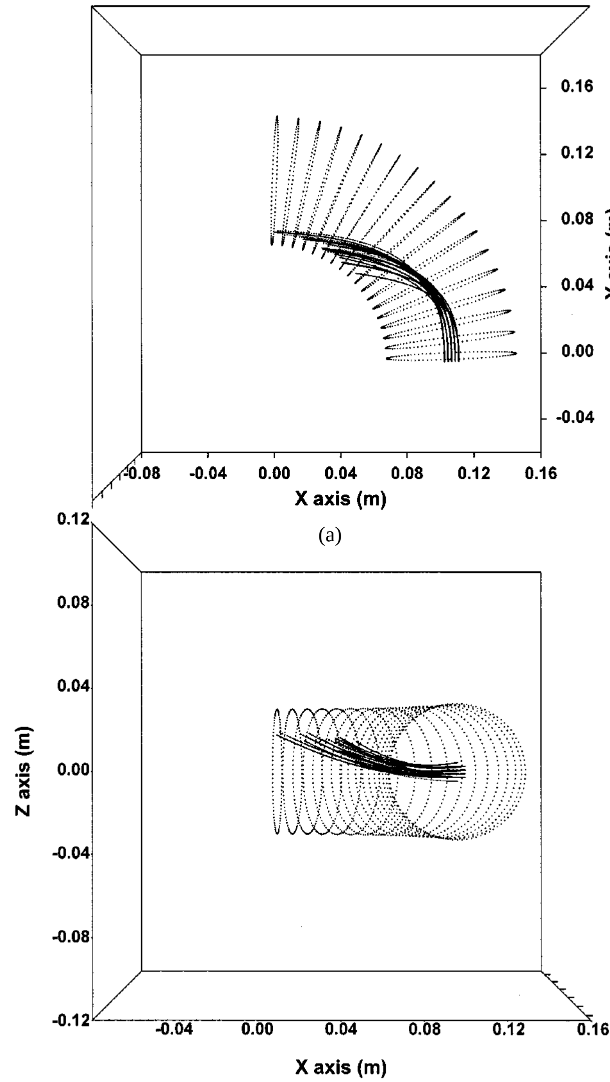
The potential of the whole duct wall and bias plate is equal to zero. The trajectories of the Ti^{+} ions at a magnetic field of 0.25 T at the center of the filter duct are depicted in Fig. 2(a) and (b). In Fig. 2(a), the trajectories are observed from the top along the XY plane, but in Fig. 2(b), they are observed from the along the XZ plane. It is seen that the magnetic field is not evenly distributed inside the duct volume and cannot guide the ions through the duct. The ions deposit on the bottom of the outer region of the filter duct. When the magnetic field is raised to 0.5 T as measured at the center of the filter duct, all the ions



(a)

(b)

Fig. 7. Trajectories of the Ti^{2+} ions at 20 V bias voltage and 0.048 T magnetic field at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane.



(a)

(b)

Fig. 8. Trajectories of the Ti^{2+} ions at 30 V bias voltage and 0.048 T magnetic field at the center of the filter duct: (a) viewed from the top along the XY plane and (b) viewed from the side along the XZ plane.

manage to pass through the filter duct as shown in Fig. 3. The ions exit downward away from the center axis out of the filter duct. At higher magnetic field, the ions will orbit inside the filter duct since they are more confined. The trajectories of the Ti^{3+} ions at 0.5 T are depicted in Fig. 4, and all the ions pass through the filter duct. The Ti^{3+} ions are more confined than the Ti^{+} ions. They orbit more frequently and exit the duct at a more centered position than the Ti^{+} ions. The computed charge state fraction, mean-charge-state, and throughput percentage of ions are plotted in Fig. 5. In this calculation, we use the prefilter percentage ratio $Ti^{+} : Ti^{2+} : Ti^{3+} = 11 : 75 : 14$ [13]. The Ti^{3+} ions saturate at its pre-filter value below 0.2 T whereas the Ti^{2+} and Ti^{+} ions saturate at higher magnetic field strength of 0.26 T and 0.5 T. The computed mean charge state is higher than the pre-filtered value and gradually drops to the initial value as the magnetic field is increased. The throughput of the ions gradually increases since more ions are saturated at higher magnetic field strength.

B. Bias Plate Influence

The trajectories of the Ti^{2+} ions at 10 V bias voltage are displayed in Fig. 6. The magnetic field strength at the center of the duct is 0.048 Telsa. The bias plate covers half of the area of the outer duct wall. The ions do not pass through the filter duct and intersect the wall at the middle of the duct near the bottom. When the bias is increased to 20 V, all the ions pass through the filter duct along its center axis as shown in Fig. 7. Only a few ions deviate from the majority and exit at the top of the duct. However, as the bias is raised to 30 V, none of the ions can escape as shown in Fig. 8. The ions are over-deflected and deposit at the edge of the filter duct near the top. The ion trajectories are different from for high magnetic field shown in Figs. 3 and 4. They traverse a straight path without orbiting. The computed charge state fraction, mean-charge-state, and throughput percentage of ions are plotted in Fig. 9. As shown, the throughput of different ions is maximized at different bias voltage depending on their charge states and is lower for higher charge state. The

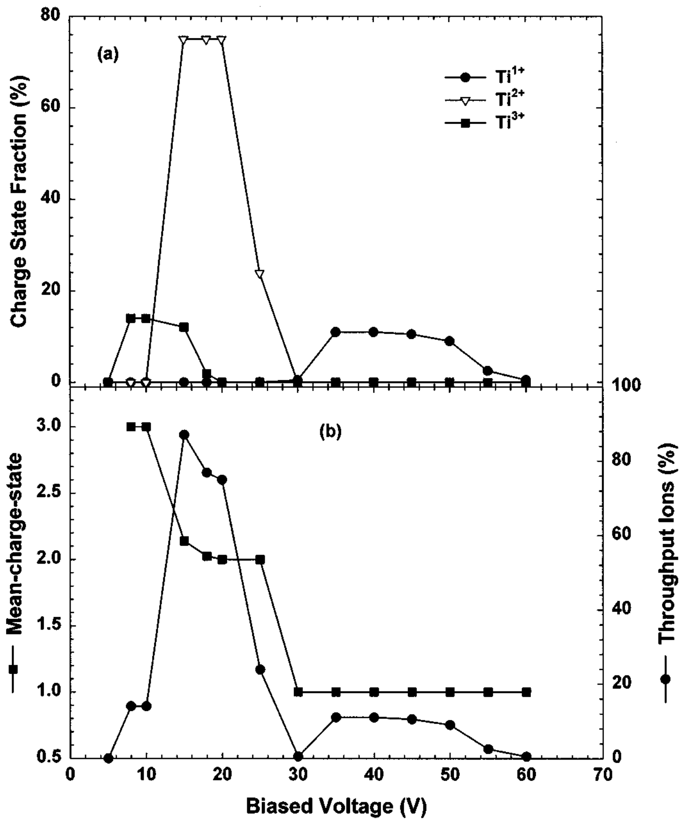


Fig. 9. Computed charge state fraction, throughput flux, and mean charge state of the transported Ti ion plasma as a function of the bias voltage.

ions can only pass through the filter duct within a narrow range of bias voltage. The voltage range for Ti^{+} does not overlap those of the other two charge state species. The computed mean charge state has a value of $+3$ at around 10 V and gradually drops to $+1$ as the bias voltage exceeds this range. The sum of the three single peaks shown in Fig. 9(a) displays two broad peaks in Fig. 9(b). Above 30 V, no Ti^{2+} and Ti^{3+} ions can pass through the filter duct.

V. Discussion

The gyration radius of a charged particle in a magnetic field can be written as [19]

$$r_{ci} = \frac{mv_\perp^2}{|qv_\perp B|} \tag{7}$$

where $v_\perp$ is the ion speed perpendicular to the magnetic field B. Equation (7) is a simplified form of (4) expressing the condition of ion confinement at constant magnetic field. However, the trajectories of the ions can only be obtained by (4). To confine a singly charged Ti ion of speed 1.5×10^4 m/s within a radius of 0.035 m, a magnetic field strength of 0.215 T is required, and only one-third of the magnetic field strength around 0.072 T is needed to confine a triply charged Ti ion. Therefore, we expect the total throughput of the higher charge state ions will saturate earlier at lower magnetic field than the lower charge state ions. The mean charge state of the throughput ions will accordingly have a higher value at lower magnetic field and gradually drop to the prefiltered value at higher field strength. The magnetic field strengths at the center of the filter duct needed to confine the Ti ions are much higher than the values obtained from (7). This is because the magnetic field strength is not uniform along the length of the duct. The field strength at the duct wall at both ends is only half of that measured at the center of the filter duct, and thus the average magnetic field strength is less than the measured value at the center of the duct.

The magnetic field strength used in the simulation in Section IV-B is 0.048 T and is not strong enough to confine the ions. According to equation (7), to confine a singly, doubly, and triply charged Ti ion of speed 1.5×10^4 m/s within a radius of 0.035 m, a magnetic field strength of 0.215 T, 0.1075 T, and 0.072 T, (respectively) is required. Therefore, without fully magnetized ions, the combined electric and magnetic field will not provide $E \times B$ drift to the ions. The electric field created by the positive potential of the inserted bias plate will only deflect the ions from the outer region to the center. However, unlike the case of applying magnetic field, applying a high electric field will not confine the ions. The ions will be over-deflected and forced to intersect the wall at the inner region of the filter duct. Therefore, the aforementioned bias voltage ranges result. Ions with a higher charge stage will experience a stronger electric force and the range will occupy the lower voltage region. As the bias voltage is increased, the mean charge state will gradually drop to lower values. It is obvious that the total throughput ions will pass through a maximum since it is a combination of the three narrow peaks. We have experimentally observed a continuous drop in the mean charge state and a maximum as the bias is increased as shown in Fig. 1(b). However, the narrow voltage ranges are not obvious in Fig. 1(a). The magnetized electrons will create an internal electric field attracting the positive ions to the center axis. In this way, the plasma electrons will maintain a background of throughput ions for different charged states. This explains the fact that a certain percentage of throughput ions are observed at a magnetic field lower than the confining field strength calculated by (7).

VI. Conclusion

We have experimentally and numerically investigated the ion charge state fractions, mean charge state, and flux of ions transmitted through a filter duct as a function of magnetic field strength and bias voltage for a multiply charged Ti plasma. The internal plasma electric field has been neglected in our simulation by assuming zero ion and electron density. The trajectories of individual ions have been determined.

Our simulation is in line with the TOF experimental results in that the mean charge state is higher than the pre-filtered value and gradually drops to the initial value as the magnetic field strength is increased. The Ti^{3+} ions will execute a greater number of gyro-orbits than the Ti^{+} ions inside the duct. Therefore, the chance of a charge state change is higher for Ti^{3+}. At very high magnetic field, the mean-charge-state (TOF) is significantly lower than the unfiltered value. Moreover, the throughput gradually increases since more ions are saturated at higher magnetic field strength. The magnetic field strength required for the ions to pass through the filter duct, as determined by the simulation, is around 0.2 to 0.5 Telsa. However, the experiments show that many ions are transported through the duct at just 0.048 T, demonstrating that the internal plasma electric field provides a background of ions of different charge states. The effect of the internal field can decrease the magnetic field strength needed to provide good ion transport by several orders of magnitude.

Since the combined electric and magnetic field structure is not sufficient to induce significant $E \times B$ drift to the ions, the electric field will only deflect the ions from the outer region to the center. Therefore, as the bias voltage increases, the mean charge state will gradually decrease and there is a maximum in the ion flux. These results are confirmed by the TOF experiments. Our results show that vacuum duct plasma phenomena such as the reduction of mean charge state at high magnetic field strength and bias can be explained in terms of standalone multiply charged metal ions under the influences of magnetic and electric forces inside the filter duct. The experimentally determined mean charge states shown in Fig. 1 vary by 6% when the ion throughput varies by a factor of three due to a bias voltage change from 0 to 50 V. These results are not inconsistent with the simulation because in our simulation, the effect of the internal plasma field has been neglected. The difference between the experimental results and the simulation reflects the fact that the magnetized electrons provide a background "sea" for the transport through the duct of ions of different charged states. At lower plasma density, around an order of magnitude less than the experimental value here of $\sim 10^{12}$ cm^{-3}, the electric and magnetic field strength will be comparable with the internal plasma field and our simulated results without the influence of electron charge will be more accurate.

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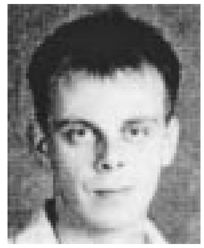

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