DYNAMICS OF MACROPARTICLE IN A WEAKLY COLLISIONAL PLASMA

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The transport of a macroparticle (MP) in an expanding cathodic vacuum arc plasma, which interacts with a background gas, is investigated. The influence of ion-neutral collisions on MP is studied in the framework of self-consistent model based on the fluid approach and orbital motion limited theory. It is found that the electrostatic reflection of MP increases with collisionality as a consequence of the increased negative potential of MP. A comparison of the ion drag and neutral drag forces governing the MP dynamics is made. It is shown that the ion drag force decreases with the ion collisionality, while the neutral drag force increases.

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INTRODUCTION

Cathodic arc plasma is produced at micron-sized, non-stationary cathode spots. Cathode erosion processes include emission of ions, macroparticles (MPs) and small fraction (<1 %) of neutral atoms [1-3]. The mass of cathode material in the form of MPs is about the same order or even greater than that of ions. The MPs occur in the range of size from fraction to tens of microns and have velocities from tens to hundreds of meters per second. The interaction of the expanding arc plasma with background gas affects the plasma chemistry, the ion composition, the ion energies and ion currents [4]. The increase in gas pressure causes an increase in gas ion fraction as well as a decrease of metal ion charge states [5]. Charge exchange collisions of multiply charged metal ions with neutrals are relevant for the reduction of the average ion charge states. The ion-neutral collisions become pronounced, when the ion mean free path is comparable with the chamber size. It is expected that the ion-neutral collisions can also affect the MP behavior.

When the MP is immersed into the plasma, it is charged via collecting the electron and ion fluxes flowing onto MP surface. The ion flux onto MP surface depends on the ratio between the plasma screening length and the ion mean free path λ/λ_j, which is called the ion collisionality. Two basic analytical approaches have been employed to calculate the ion fluxes onto MP immersed into the weakly collisional (WC) plasma. The orbital motion limited (OML) theory is applicable when the plasma screening length λ is much larger than the radius of MP and collisions are rare [6]. The OML theory neglects the ion collisions with neutrals. In the framework of the collision enhanced collection (CEC) theory, the charge exchange collisions affect the ion flux [7]. The CEC theory is suited when the ion collisionality $\lambda/\lambda_j \geq 0.1$.

We have recently considered the effect of ion collisionality on the charging of MP in the cathodic arc sheath [8]. In the present work, we analyse the charging of MP as well as the contribution of the various forces acting on MP in the interelectrode region of the cathodic vacuum arc operated in low-pressure nitrogen atmosphere. The plasma model accounts for the non-resonant charge exchange between the multiply charged metal ions and neutrals. The generation of gas ions is assumed to be due to both the charge exchange and the electron impact ionization.

1. PLASMA MODEL

The plasma model describes the interelectrode region of the cathodic vacuum arc, which extends from the cathode spot plasma to the anode sheath. The plasma consists of electrons, j species of metal ions (M^+, M^{2+}, M^{3+}), i reactive gas species (N_2^+, N^+), with a uniform background neutral gas. The metal ions of j-th species have temperature T_j and mass m_j. The electrons and gas ions have thermal velocities $\upsilon_{Te} = (8k_BT_e/\pi m_e)^{1/2}$ and $\upsilon_{Ti} = (8k_BT_i/\pi m_i)^{1/2}$, respectively. Here, $T_{e,i}$ and $m_{e,i}$ are the temperature and mass of electron and gas ion, respectively, and k_B is the Boltzmann constant.

Charge exchange processes change the charge of metal ion from Z to $Z-1$

$$M^{Z+} + N_2 \Rightarrow M^{(Z-1)+} + N_2^{\ +},\ \ Z = 1, 2, 3. \quad (1)$$

The plasma originates from the cathode, and the x axis is directed from the cathode to the anode. In the steady-state, the continuity equations for metal ion species are as follows:

$$\frac{d}{dx}\left(n_j u_j\right) = S_{j+1} - S_j, \quad j = 1, 2, 3. \quad (2)$$

where n_j and u_j are the density and velocity of metal ions, respectively; S_{j+1} denoted symbolically the source term of ions of j-th species, S_j denoted the sink term of ions of j-th species. For inelastic collision mechanism just described, the collision term S_j for the ions can be expressed as $S_j = nn_j\langle\sigma_j u_j\rangle$, where n is the particle density of neutral background gas.

The cross section σ_j for charge exchange between metal ions of type j and neutrals increases with the ion charge state number Z quadratically [9]

$$\sigma_j\,[cm^2] = 0.88\times10^{-16} Z^2\left(I_H/I\right)^2, \quad (3)$$

where I and I_H are the ionization potential of the target particle and the hydrogen atom, respectively.

In contrast to metal ions, the gas ions are produced by charge exchange as well as by electron impact ionization [10]. Thus, the continuity equation for gas ions is

$$\frac{dn_i}{dx}(n_i\upsilon_i) = k_{ion}n_e n + \sum_{j=1}^{3} S_{j+1} - \sum_{j=1}^{3} S_j\,, \quad (4)$$

where n_i is the density of gas ions, respectively; n_e is the particle density of electrons.

The rate coefficient of electron-impact ionization of gas k_{ion} in the case of a Maxwellian distribution of electrons is given by [11]

$$k_{ion} = C_i\upsilon_{Te}(1+2k_BT)\exp(-I/k_BT_e). \quad (5)$$

For N_2, I=15.58 eV, C_i=0.85×10^{-16} cm^2eV^{-1}.

The momentum equation for metal ions is

$$u_j\frac{d}{dx}(n_ju_j) + n_ju_j\frac{du_j}{dx} + n_ju_j\nu_j = 0\,, \quad (6)$$

where q_α is the ionic charge, $\nu_\alpha=n\sigma_\alpha u_\alpha$ is the collision frequency. Taking $\nu_j=u_j/\lambda_j$, where λ_j is the mean free path, and noting that the ion flux $J_j=n_ju_j$, this equation can be rewritten

$$\frac{du_j}{dx} = -u_j\frac{d}{dx}\ln J_j - \frac{u_j}{\lambda_j}. \quad (7)$$

The equations (2), (5), and (7) can be made dimensionless by introducing the following variables

$$z \equiv \frac{x}{\lambda_D}, \alpha_j \equiv \frac{\lambda_{De}}{\lambda_j}, \tilde{u}_j \equiv \frac{u_j}{c_j}, \tilde{J}_{j,i} \equiv \frac{J_{j,i}}{n_0c_s},$$

$$K_{ion} \equiv \frac{k_{ion}n_en\lambda_D}{n_0c_s}, \tilde{S}_j \equiv \frac{S_j}{n_0c_s}, \quad (8)$$

where $c_j=(k_B\,T_e/m_j)^{1/2}$ is the sound velocity of j-th ion species, $\lambda_{De}=(\varepsilon_0T_e/n_0e^2)^{1/2}$ is the electron Debye length. The key parameter is ion collisionality α_j which relates to the background gas pressure p as

$$\alpha_j = \lambda_{De}n\sigma_j = \frac{\lambda_{De}p\sigma_j}{k_BT_g}, \quad (9)$$

where T_g is the gas temperature.

As a consequence of the proposed scaling, the governing equations become

$$\frac{d}{dz}\tilde{J}_j = \tilde{S}_{j+1} - \tilde{S}_j, \quad j=1,2,3, \quad (10)$$

$$\frac{d\tilde{u}_j}{dz} = -\tilde{u}_j\frac{d}{dx}\ln\tilde{J}_j - \alpha_j\tilde{u}_j\,, \quad (11)$$

$$\frac{d}{dz}\tilde{J}_i = K_{ion} + \sum_{j=1}^{3}\tilde{S}_{j+1} - \sum_{j=1}^{3}\tilde{S}_j\,. \quad (12)$$

The set of equations (10)-(12) is a closed system of equations. All plasma parameters depend only on the dimensionless distance from the cathode z.

2. MP CHARGING

The MP of radius a immersed in the cathodic arc plasma is charged due to collecting the electrons as well as metal and gas ions from the plasma. The floating potential ϕ_d of MP is determined by the balance of electron current I_e and sum of ion currents:

$$I_e(\phi_d) = \sum_j I_j(\phi_d) + \sum_i I_i(\phi_d). \quad (13)$$

The MP charge Q is related to the MP potential as

$$Q(z) = C\phi_d(z)\,, \quad (14)$$

where $C=4\pi\varepsilon_0a$ is the capacitance of the MP.

The OML theory [6] can be used to calculate electron and ion currents. The OML theory is applicable if

$$a \ll \lambda \ll \lambda_j\,. \quad (15)$$

In the plasma with supersonic ions, the ions cannot contribute to shielding. Therefore, the plasma screening length λ is very close to the electron Debye length λ_{De} [12].

In the case of Maxwellian electrons and negatively charged MP, the electron current is determined as:

$$I_e = \pi a^2en_e(z)\upsilon_{Te}\exp\left(\frac{e\phi_d(z)}{k_BT_e}\right). \quad (16)$$

The currents of gas ions are

$$I_i = \pi a^2q_in_i(z)\upsilon_{Ti}(z)\left(1-\frac{e\phi_d(z)}{k_BT_i}\right). \quad (17)$$

The velocity distribution function of metal ions of each species is approximated by a shifted Maxwellian distribution. Therefore, the currents of metal ions can be written as:

$$I_j = \pi a^2q_jn_j(z)\upsilon_j(z)\left(1-\frac{2q_j\phi_d(z)}{m_j\upsilon_j^2(z)}\right), \quad (18)$$

where the total mean velocity and corresponding energy of ions are given in [13]

$$\upsilon_j(x) = \left(u_j^2 + \frac{8k_BT_j}{\pi m_j}\right)^{1/2}, \quad (19)$$

$$\frac{m_j\upsilon_j^2}{2} = \frac{4k_BT_j}{\pi} + \frac{m_ju_j^2}{2}. \quad (20)$$

3. MP DYNAMICS

The total force acting on a MP during its motion to the substrate is

$$\vec{F} = \vec{F}_E + \sum_j\vec{F}_{dj} + \vec{F}_{dn}\,, \quad (21)$$

where $F_E=QE$ is the electric force, F_{dj} is the ion drag force caused by the momentum exchange between the metal ion of type j and MP, and F_{dn} is the neutral drag force caused by the momentum exchange between the neutrals and MP. The ion and neutral drag forces are main forces acting on MP in the bulk plasma.

The ion drag force consists of a collection force and an orbit force. For high velocities such as metal ion velocities, the collisionless ion drag is purely determined by the ion collection [14]

$$\vec{F}_{dj} = \pi a^2n_jm_j\upsilon_j\vec{u}_j\left(1-\frac{2q_j\phi_d}{m_j\upsilon_j^2}\right). \quad (22)$$

Gas ions have no directed velocities, and, therefore, they don't contribute to the total ion drag. Ion drag force accelerates the MP towards the plasma boundaries.

In contrast to the ion drag force, the neutral drag force results in a deceleration of MP. When the relative velocity between the MP and neutrals is very small compared to the neutral thermal velocity $\upsilon_{th,n} = (8k_B T_g / \pi m_n)^{1/2}$, the neutral drag force is given by the Epstein expression [15]:

$$\vec{F}_{dn} = -\frac{8}{3}\sqrt{2\pi}\, a^2 n m_n \upsilon_{Tn} \vec{V}, \qquad (23)$$

where V is the MP velocity. Since the neutral drag is directly proportional to neutral gas density n, increasing the gas pressure results in strengthening this force.

4. RESULTS AND DISCUSSION

In order to consider the influence of the collisions on the MP dynamics in the cathodic arc, it is necessary to couple the MP model with the plasma model. Therefore, the first step in the present work is the modeling of the interelectrode region. The plasma parameters of titanium arc operated in nitrogen are: the electron temperature T_e =2 eV, the plasma bulk density $n=10^{16}$ m^{-3}, the temperature of titanium ions is about 0.3 eV, and both temperatures of nitrogen ions and neutrals are kept at room temperature (0.026 eV). These parameters are typical for cathodic vacuum arc plasma, used in TiN deposition.

According to the approximation (3), the cross sections of the charge exchange reactions of Ti^+, Ti^{2+}, Ti^{3+} ions in nitrogen are $\sigma_1 = 6.5\times10^{-17}$ cm^2, $\sigma_2 = 2.6\times10^{-16}$ cm^2, $\sigma_3 = 5.9\times10^{-16}$ cm^2, respectively. According to formula (9), the resulting degrees of collisionality for Ti^+, Ti^{2+}, Ti^{3+} are $\alpha_1 = 1.6\times10^{-4}\,p$, $\alpha_2 = 6.3\times10^{-4}\,p$, $\alpha_3 = 1.4\times10^{-3}p$ (p in Pa). The dependencies of the normalized ion fluxes on the number of collisions are presented in Fig. 1. Examining the Fig. 1, the flux of Ti^{3+} ions decreases practically to zero because the Ti^{3+} ions have larger cross section compared with those of Ti^{2+} and Ti^+ ions. The flux of Ti^+ ions initially increases with increasing the number of collisions due to charge transfer reactions of the Ti^{2+} ions. Then, the annihilation of Ti^{2+} and Ti^{3+} ions populations occurs, resulting in the decrease in Ti^+ counts.

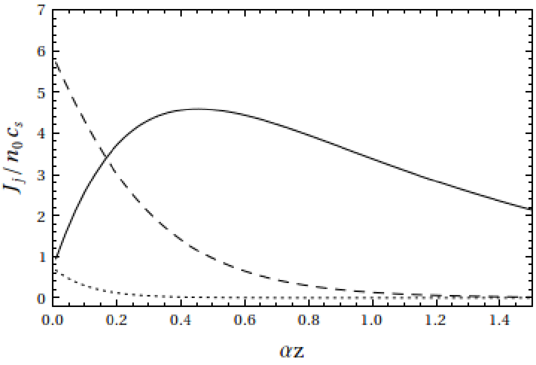

Fig. 1. Dependence of the normalized ion flux on the number of collisions: Ti^+ (solid line), Ti^{2+} (dashed line), Ti^{3+} (dotted line)

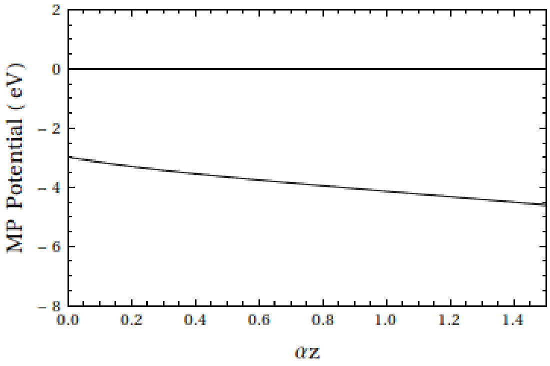

Fig. 2. Dependence of the MP potential on the number of collisions

As the ion collisionalities are very small for the pressure range of interest (≈ 1.5 Pa or less) the OML theory is applicable to calculate the MP potential. The MP potential obtained from the current balance (13) is shown in Fig. 2. It is seen that the ion-neutral collisions increase the negative potential of MP. These results can be explained by the decreasing of the ion current density with the distance and the pressure. The MP potential weakly depends on the ion charge state.

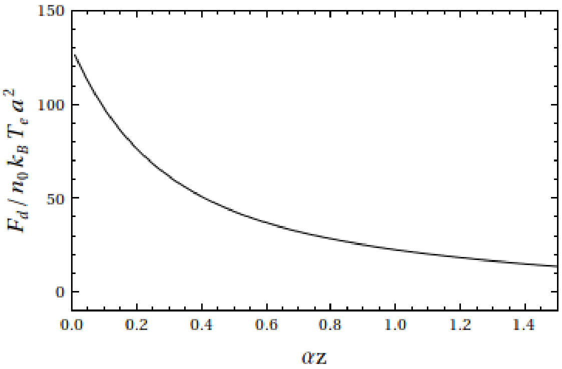

Fig. 3. Dependence of the normalized ion drag force on the number of collisions

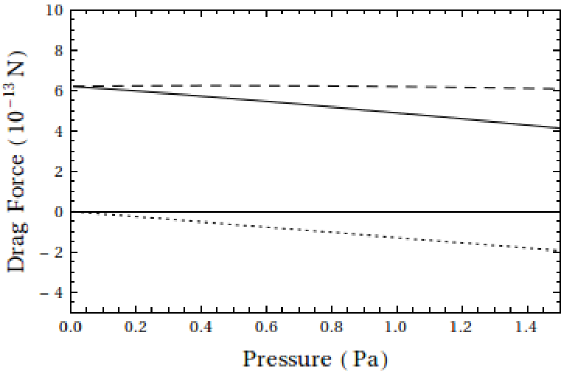

Fig. 4. Dependence of the ion drag force (dashed line), neutral drag (dotted line), and total force (solid line) on the pressure

Fig. 3 shows the dependence of the normalized ion drag force on the number of collisions. The ion drag force decreases with the collisions since it depends on the ion fluxes and ion velocities, which decrease with the collisions too. The ion drag force can compete with the neutral drag force. We consider, as an example, the forces acting on MP with radius 0.1 μm and velocity of 10 m/sec at distance 0.1 m from the cathode. For comparison, the ion drag and the neutral drag are plotted on the same Fig. 4. At pressure 1.5 Pa, the neutral drag force, which opposes the MP's motion, is twice less than the ion drag force.

CONCLUSIONS

The effect of collisionality on MP placed in a flowing collisional cathodic arc plasma is investigated.

It is found that the ion collisionality reduces the ion drag force, which accelerates the MP toward the boundaries of plasma. On the other hand, the neutral drag force, acting in the opposite direction, increases with the collisionality. The electric force associated with MP charge is small in the bulk plasma. However, it becomes larger near the sheath edge. The electrostatic reflection of MP increases with collisionality as a consequence of the increased negative potential of MP. All forces can balance near the sheath edge, and, hence, a MP can be confined.

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ДИНАМИКА МАКРОЧАСТИЦЫ В СЛАБОСТОЛКНОВИТЕЛЬНОЙ ПЛАЗМЕ

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Исследован транспорт макрочастицы (МЧ) в расширяющейся плазме катодной вакуумной дуги при взаимодействии с газом. Влияние столкновений ионов с нейтралами на МЧ изучается в рамках самосогласованной модели, основанной на гидродинамическом подходе и теории ограниченного орбитального движения. Получено, что электростатическое отражение МЧ увеличивается со столкновительностью вследствие увеличения отрицательного потенциала МЧ. Проведено сравнение силы ионного увлечения и силы трения со стороны нейтралов, которые определяют динамику МЧ. Показано, что сила ионного увлечения уменьшается со столкновительностью, в то время как сила трения со стороны нейтралов увеличивается.

ДИНАМІКА МАКРОЧАСТИНКИ В ПЛАЗМІ ЗІ СЛАБКИМИ ЗІТКНЕННЯМИ

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Досліджено транспорт макрочастинки (МЧ) у плазмі, що розширюється, катодної вакуумної дуги при взаємодії з газом. Вплив зіткнень іонів з нейтралами на МЧ вивчається на підставі самоузгодженої моделі, що базується на теорії рідини та теорії обмеженого орбітального руху. Отримано, що електростатичне відбиття МЧ зростає із зіткненністю внаслідок збільшення від'ємного потенціалу МЧ. Зроблено порівняння сили іонного захвату та сили тертя з боку нейтралів, які визначають динаміку МЧ. Було показано, що сила іонного захвату зменшується із зіткненністю в той час, як сила тертя з боку нейтралів збільшується.