Monte Carlo calculation of the energy parameters and spatial distribution of the cathodic arc ions while passing through the macro-particles filters

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Abstract: The flow, energy distribution and concentrations profiles of Ti ions in cathodic arc are studied by test particle Monte Carlo simulations with considering the mass transfer through the macro-particles filters with inhomogeneous magnetic field. The loss of ions due to their deposition on filter walls was calculated as a function of electric current and number of turns in the coil. The magnetic field concentrator that arises in the bending region of the filters leads to increase the loss of the ions component of cathodic arc. The ions loss up to 80% of their energy resulted by the paired elastic collisions which correspond to the experimental results. The ion fluxes arriving at the surface of the substrates during planetary rotating of them opposite the evaporators mounted to each other at an angle of 120° characterized by the wide range of mutual overlapping.

Keywords: coatings, particles, Monte Carlo, stochastic, cathodic arc.

1 Introduction

Cathodic arc physical vapor deposition (CA-PVD) method allows obtaining the coatings, which are characterized by high hardness, density and adhesion strength to a substrate [1–5]. However, one of the disadvantages of this method is a droplet formation due to a cathode spot operation [6]. For instance, these droplets are observed for such popular coating elements, as titanium and chromium [7, 8]. Different filters (generally based on a magnetized plasma in an electromagnetic field in a curvilinear separator) are applied to prevent the droplet deposition on a coating surface [6]. When CA-PVD is sensitive to experiment conditions, parameters of a separator and magnetic field influence on the spatial distribution of plasma flow, thereby changing coating structure and properties. Consequently, the prediction of plasma flow parameters is an important step in the process of coating development and production.

The aim of this work was to develop the mass transfer model of the plasma through the droplets filter and study the plasma flow on the substrate with a planetary rotation.

2 Methods

The mass transfer calculation of Ti^{2+} flow through the magnetic filter (in the shape of a torus with a turn angle α of 120°, as shown in figures 1) was accomplished by the Monte Carlo method. The initial site of ions was set by generating a random coordinate, which also considers the influence of magnetic fields. This influence of magnetic fields is the preferential sputtering of a cathode at an angle γ with the shift of cathode spot to the internal wall, as shown in figure 1.
In addition to the initial site, the ion flow is also given by charge (Z) and velocity (V), whose distribution described by Maxwell equation [10, 11]. The velocity and charge of Ti$^{Z+}$ were established according to the experimental data obtained by the authors of the works [11].

Figures 1. Geometric parameters of chamber and schematically representation of cathodic spot erosive impact

Since the contribution of inelastic collision (associated with the excitation of internal states of gas atoms) in the energy dissipation of the ion is negligible [12], only elastic collision was considered. In addition to the inelastic collision, plasma characterized by recombination process of ions and neutral atoms. It is known, that recombination process slightly affects the plasma charge distribution than the time of flight less than $10^{-2}$ s [12]. When the velocity of ion in the cathodic arc equal to $10^4$ m/s [10–13], the average time of flight from the cathode spot to substrate in the $\pi$-position approximately equal to $10^{-4}$ s, thus we enter the assumption of recombination process absence in our calculation. Modified Born-Mayer potential $U_{BM}$ and quasi-hard spheres [14] were used for the calculation of cross section $\sigma$, mean free path $\lambda$ and angle of scattering $\Theta$ between atoms with the atomic numbers $Z_1$ and $Z_2$, which is given by (1) [14]:

$$U_{BM} = 95.863(Z_1Z_2)^{0.7383} \exp \left( \frac{-r}{0.122(z_1^{0.0387} + z_2^{0.0387})} \right)$$  (1)

3 Results

3.1 Ions energy distribution

According to the calculation, the ion loss equal to 92 % that correlated with experimental results [12]. This ion loss was practically independent of the magnetic field parameters, which regulated by the current in coils from 5 to 20 A.

Results of Ti ion energy calculation are shown in figure 2. As it shown, the average energy of ion flow decreased by 17 % after the ions had passed the filter, which is correlated with Ref. [15]. Since reactive gas added to chamber fills all volume of the chamber (including separator), it decreases the mean free path of ions, resulting in the ion energy scattering. Is should be noted that the loss of energy from the initial energy of ions in relative values by low-energy ions predominates over the same losses of high-energy ions. This phenomenon can be related with the difference in the mean free path, as shown in figure 3. Thus, the lower energy of ions, the more collision acts it undergoes, which means the low-energy ions dissipate more energy.
Figure 2. Ion energy distribution (1) in cathode spot and (2) at the virtual probe

Figure 3. Influence of ion energy on the mean free path

Figure 4 shows the ion intensity distribution on the virtual probe (see probe in fig. 1). As can be seen, approximately 80 % of ions shifted from a filter axis to internal wall of the filter. This shift caused by several factors. First, the evaporation of cathode at an angle $\gamma$ leads to preferential sputtering of cathode area, which located on the left side. Second, the coil density of a wall with a low torus radius exceeds the one with the high torus radius; as a result, a magnetic field concentration magnetizes the plasma to the internal wall of the filter.

Figure 4. Ion density distribution at the virtual probe

3.2 Concentration profiles

Properties of coatings, obtaining by a multisource mode physical vapor deposition, depend on a structure and structure parameters as well as an elemental composition. In the case of multilayer coatings, some of these parameters are a modulation period and structure of layer interface. Consequently, it is important to define the distribution of the ion flow as the function of a substrate position related to the evaporators, since the ion flow on the substrate influence on the modulation period. In this work, the calculation of ion distribution in the chamber was done, whose results are shown in figure 5. As can be seen, the ion flow characterized by the non-uniform distribution and asymmetry of the ion density related to a 0-$\pi$ axis due to the strong magnetic field generated by filter coil, which based below this axis.

Figure 6 shows the distribution of the ion flow density as the function of the substrate position (as illustrated in fig.1 and 5). As can be seen, the ion flow shifted from the filter axis to the left side and can be described by the sines law [16] with some asymmetry of a peak, due to the non-uniform of the ion flow. At the same time, the distribution of the ion flow on the substrate is smoothed as the substrate is moved in height from the center of the plasma flow cross section. It should be noted that there is no noticeable redistribution of the ion energy both in position 0 and
in position π, which can be connected with exceeding the ion mean free path over the geometric parameters of the chamber.

**Figure 5.** Contour map of the plasma distribution in the chamber

In the case of the planetary rotation of the substrate with the ratio of the angular speed of a substrate rotation around own axis to the angular speed of the substrate rotation around the axis of the table as 9:1, it occurs shading the plasma flow. This shading leads to the formation of nine concentration peaks, as it shown in figure 7. According to the calculation of two cathode and three cathode systems, the plasma flows from cathodes overlap each other with the formation of two-level structure without of a «death» zone in contrast to Ref. [16].

**Figure 6.** Density of the ion flow on the substrate at different height (in sm)

**Figure 7.** Density of the ion flow on the substrate with planetary rotation

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4 Conclusion

The mass transfer of the ion flow through the magnetic filter of micro particles was calculated. It was found what the non-uniform magnetic field leads to shifting of the ion flow to internal wall of separator. In consequence, the ion flow distribution in the chamber also characterized by asymmetry. The planetary rotation of substrates provides the formation of two-level structure with overlapping the ion flow from different cathodes in the case of multicomponent mode.

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