Modelling of cathodic arc PVD plasma flow in separator with non-uniform magnetic field

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Abstract. A computer model of the Monte Carlo mass transfer of vacuum arc plasma through a magnetic separator of the dropping phase was developed and the calculation was made for a titanium cathode. It has been established that as a result of passing through the separator, titanium ions lose about 17% of energy due to elastic collisions, while less charged ions are subject to large relative energy losses. The calculated loss of the ionic component on the chamber walls is 90% that corresponds to the experimental observations. A non-uniform magnetic field leads to a shift of the plasma flow to the walls of the separator, however, the position of the substrates along the height makes the greatest contribution to the unevenness of the concentration flow. It has been established that during the planetary rotation of the substrates, the overlap areas of the plasma flows are insignificant, while the plasma flow is present in all parts of the substrate motion, without the appearance of “shadow” zones.

1. Introduction
Nowadays, various methods of physical vapor deposition are commonly used in industry for various purposes, such as increasing the service life of products, functional properties, as decorative coatings [1–5]. However, one of the drawbacks of this method is the formation of a droplet fraction in coatings from a cathode spot. The size of such drops can be up to several micrometers, which significantly reduces the mechanical properties of coatings [6–8]. In order to prevent droplets insertion into the coating, methods based on the plasma deflection under magnetic fields are used [6]. The use of such filters leads to a change in the concentration-energy parameters of the plasma, which affects not only the thickness of the coatings, but also the composition and structure.

The aim of this work is to develop a computer model of plasma transfer through droplet magnetic separators and calculate the concentration-energy parameters of the ion component of the titanium cathode plasma flow in the BULAT-6 installation chamber equipped with magnetic separators.

2. Methods
To calculate the plasma mass transfer and concentration-energy parameters of the ion component of the plasma flow, the Monte-Carlo computer simulation method was used. The algorithm for calculating the model is presented below:

- By generating a random number, the initial energy of the ion and its charge are set so that the energy distribution of the ions is described by the Maxwell equation and corresponds to the experimental data; The initial position of the ion is also set by generating a random number, but taking into account the preferential sputtering of the cathode at an angle $\gamma$ in the presence of a separator magnetic field [9–11].
• Virtual displacement of an ion by the value of x with an accuracy of $10^{-6}$ m of the free path of an ion in a chamber filled with argon atoms, which is calculated in the approximation of quasi-rigid spheres using the Born-Meier potential equation presented in reference [12].
• Check of the probability of an elastic collision of an ion by the results of which the ion either continues its movement until the next collision, or collides and loses some of its energy. The calculation was performed for Ti$^{2+}$ titanium sprayed in argon with a pressure of 0.8 Pa, for $10^6$ particles. Since the contribution of inelastic collisions to the energy dissipation is insignificant [14], only elastic collisions were taken into account. In addition, taking into account the geometrical dimensions of the chamber of vacuum ion plasma plasma deposition from the gas phase, the average time of flight from the cathode surface to the chamber walls or substrate holders is less than $10^{-4}$ s [10–13], which makes it possible to ignore recombination processes in the computer model.

![Figure 1. Schematic representation of the BULAT-6 unit, equipped with a droplet phase magnetic separator and rotating substrate holder.](image)

3. Results and discussions

3.1. Energy parameters of the plasma flow

According to the calculations, the loss of plasma flow components on the walls of the separator chamber is 90%, which corresponds to the experimental data. Moreover, these losses practically do not depend on the magnitude of the magnetic field, which are controlled by the value of the current in the magnetic coils in the range from 5 to 20 A.

The results of the energy parameters of the titanium ion plasma are presented in figure 2. It can be seen that, on average, the ion energy decreases by 17% after passing through the magnetic separator, which corresponds to the experimental data [15]. These losses are mainly caused by the scattering of titanium ions on argon atoms. It should be noted that in relative terms, ions with low energy dissipated more energy than highly charged ions, due to the difference in the free path. In figure 3, it can be seen that the mean free path for high-energy ions was approximately 0.3–0.5 of the total span of the individual ion. Consequently, such ions underwent up to 6 energy scattering events, while for ions with an energy of 50 eV, the number of such acts exceeded on average 16.

Figure 4 shows the intensity distribution of the ion flux as a function of the position on the virtual probe, which was installed at the outlet of the droplet separator. As can be seen, more than 80% of the ions are displaced from the axis of the separator to the internal chamber of the separator. This offset is due to several reasons. First, the predominant sputtering of the cathode at an angle $\gamma$ leads to the sputtering of the cathode region adjacent to the side of the separator with the highest density of turns of the magnetic coil. Secondly, the concentration of magnetic fields, due to the different density of the turns, form a magnetic field with an uneven distribution of lines of force relative to the axis of the separator. This leads to different magnetization of the ionic component of the plasma flow.
3.2. Plasma flow distribution

Since the properties of coatings depend not only on the nature of their material, but also on their structure, it is important to take into account the concentration parameters of the plasma flow in the processes of vacuum arc deposition of coatings in unit equipped with several evaporators. Parameters such as plasma flux density, substrate rotation speed and their position relative to evaporators determine the modulation period of the coating, the structure of the interface between the layers, and also indirectly affect the phase composition. In the case when the plasma flows entering the surface of the substrate overlap, the formation of multicomponent compounds proceeds in the layers based on the plasma components of these flows and the reaction gas, for example, solid solution nitrides, intermetallic compounds of different composition. If overlap of plasma flows does not occur, then the formation of such compounds is possible only at the interface of the layers. Thus, to control the growth process of a coating by this group of methods, it is important to know the plasma concentration parameters as a function of the intensity of the plasma flow from the position of the substrates. Figure 5 presents a map of the density of the plasma flow inside the chamber of a vacuum-arc installation of the Bulat type. In this case, the axis of the separator at the outlet corresponds to the axis of the chamber 0 - π. The greatest density of the plasma, as it should be expected, corresponds to the region of the exit of the plasma flow from the separator. There is also a shift in the flow with respect to the axis 0 - π, due to the uneven magnetic field generated by the magnetic coil of the droplet phase separator. As the distance from the separator increases, the plasma evenly spreads in the chamber, while the density at the point 1.5 π is slightly higher than the density at the point 0.5 π.

However, from the practical point of view, the main interest is not the plasma distribution in the chamber, but the concentration of the plasma flow on the surface of the substrates. Figure 6 shows a plot of plasma concentration on the surface of the substrate as a function of the position of the substrate in the coordinates of rotation of the substrate holder. These data correspond to the dotted line.
in figure 5. It can be seen that the vertical shift relative to the center of the chamber by 10 cm leads to a decrease in the intensity of the plasma flow by more than two times. Moreover, if at a distance from the exit of the plasma flow from the exit of the separator, the difference in intensity is practically absent, that a fourfold difference is observed near.

**Figure 5.** Plasma density map inside the chamber for the BULAT-6 unit.

Consequently, in the deposition of coatings from several cathodes of different materials, it is important to consider that not only the thickness but also the composition and structure of the coatings will vary from the level of a sample installation. In the case of planetary rotation of the substrate, with the ratio 9:1 of the rotation period around its axis to the rotation period of the substrates around the axis of the substrate holder, shading of the plasma flow also occurs, the concentration profile of which is shown in figure 7. According to the calculations for the two and three-cathode system, the coatings are formed with overlapping plasma flows without a “dead” zone, as indicated in [16].

**Figure 6.** Density of plasma flow to the surface of the substrate at different heights (in cm).

**Figure 7.** The concentration profile of the plasma flow on the surface of rotating substrates.

4. **Conclusions**

A model of mass transfer of a vacuum arc plasma by the Monte Carlo method was developed and calculated the energy parameters of plasma for a titanium cathode in an argon atmosphere at a pressure of 0.8 Pa. It was found that inhomogeneous magnetic fields of magnetic separators lead to a shift of
the plasma flow to the inner wall of the separator with a high density of turns of the magnetic coil. This inhomogeneity of the magnetic field leads to a shift of the plasma flux inside the chamber, which affects the concentration fluxes of the plasma component on the surface of the substrates. It was also demonstrated that the location of the substrates at different heights leads not only to a decrease in the intensity of the plasma flow, but also to a change in the shape of the concentration profile with a decrease in the intensity of the plasma flow in the areas corresponding to the output of the plasma flow from the separator as the mounting height of the substrates changes.

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