Bulgarian Chemical Communications, Volume 47, Special Issue B (pp. 177–181) 2015

Predicting the erosion of the cathode material in PVD systems

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Predicting the erosion of the cathode material in cathodic arc evaporation of metal in a vacuum environment is an interesting task with a variety of applications. In this paper, a method for calculating of the evaporated cathode material as a function of the arc current by which it was evaporated is presented. The method is suitable for the processes of the cathodic arc evaporation of metals in a vacuum environment from massive cathodes by DC arc. In the model has introduced a correction factor that represents the differences in technical terms of the metal evaporation process in vacuum environment by electric arc. The correction factor is determined experimentally once-through for each different type of the cathode shape. The method is illustrated by an example of arc evaporation of massive titanium cylindrical shape cathode.

Key words: PVD, vacuum arc, cathode spot

INTRODUCTION

The ability to be able to determine the evaporated quantity of the cathode material depending on the magnitude of the electric arc current in the PVD systems is crucial and it is a first step in the modeling of coatings deposition process in such systems.

Cathode erosion has been theoretically studied by various researchers using models based on the balance of energy flux and charged particles between the spot and the near-cathode region.

The topic of arc discharges has been discovered at the beginning of the 19th century, serious efforts regarding their physical explanation and especially the modeling of electrode processes did not start until one century later [1]. One of the earliest investigations of this area are the works of Langmuir [2, 3], Tonks and Langmuir [4], Mackeown [5]. As Riemann reported in [6] the basic features of the plasma-sheath transition have been revealed in the works of Langmuir [3] – especially in the famous kinetic analysis of the low-pressure column due to Tonks and Langmuir [4]. Years later Dolan and Dyke [7] and Murphy [8] presented their works "Temperature and field emission of electrons from metal" and "Thermionic emission, field emission, and the transition region", following by Lee with his works over T-F theory of electron emission in high current arcs [9], energy distribution and cooling effect of electrons emitted from an arc cathode [10], and theory of the cathode mechanism in meal vapor arcs [11], which has been turned in a base for the later works over understanding and modeling the cathode arc processes.

The theory and conception of the cathode spot, as the cathode material erosion in vacuum is wide discussed in literature by Lee in 1951, 1960, 1961 [9–11], Ecker 1963 [12], Hantzsche in 1976 [13], Lyubimov in 1978 [14], Ivanov in 1985 [15], Nazarov in 1990 [16], Puchkarev in 1990 [17], Mitterauer in 1996 [18], Gayet in 1996 [19], Jüttner in 1997 [20], Anders in 1997 [21], Coulombe in 1997 [22–24], Anders in 2001 [25], Massaad in 2006 [26], Lefort in 2012 [27].

Kimblin [28] reported that the maximum ion current is in range of 7–10% of the arc current for electrodes with DC arc current level. He has made experiments with wide number of elements in arc current range of 50–1000 A. In [29], a year later, Kimblin reported that the maximum ion current from the cathode regions is approximately 8% of the arc current. This led to the conclusion that ion currents of approximately 8% of the arc current are emitted from the cathode regions associated with arc spots on the cathode materials in general.

Coulombe [23] reported that a net positive space charge sheath, or cathode sheath, of voltage drop is formed at the plasma-cathode boundary due to the presence, in different amounts, of three charge carriers [6]: 1) the ion generated by ionization of the atoms vaporized at the cathode spot surface, accelerated back toward the cathode; 2) the Boltzmann distributed plasma electrons retro-diffusing toward the cathode; and 3) the thermo-field electrons emitted by the cathode spot surface.

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Boxman [1], Coulombe [22–24], Massaad [26] and Lefort [27] have suggested the models of the processes near to the cathode surface which are based on the knowledge the temperature of cathode spot and electrons, the material vapour pressure. Their models are quite good to understanding the processes around the electric arc and the cathode spot region, but in these cases making the mathematical modeling and simulation require additional information (the temperature of cathode spot and electrons, the material vapour pressure) to be predict the cathode erosion.

In this paper, a method for calculation of the evaporated cathode material, in PVD systems, as a function of the arc current is presented. Correction factor that represents the differences in technical terms of the metal evaporation process in vacuum environment by electric arc is introduced in the model. The method is illustrated by an example of arc evaporation of massive titanium cylindrical shape cathode.

SURFACE OF CATHODE

The main processes which occur at the cathode surface are emission of electrons and atoms. The emission process, when the temperature and the field are high, is strongly dependent on both variables, and has been named T-F emission by Dolan and Dyke [7, 9]. The electron emitted current density from the heated metal surface to the temperature T_s by the T-F emission is expressed with the Ridchardson-Dushman equation for the thermionic emission once corrected for the Schottky effect is [1, 24, 30]:

$$J_{TF} = \frac{4\pi e m_e k^2 T_s^2}{h^3} \exp\left(-\frac{e\phi_{eff}}{kT_s}\right) \tag{1}$$

$$\phi_{eff} = \phi - \sqrt{\frac{eE}{4\pi\varepsilon_0}} \tag{2}$$

where: m_e and e are the mass and charge of the electron, k and h are the Boltzmann and Planck constants, ϕ_{eff} and ϕ are the effective work function and the work function of the cathode material, ε_0 is the permittivity of vacuum, and E is the electric field near to the cathode surface.

The total current density J_T on the cathode surface is composed of three parts [1]:

$$J_T = J_i + J_e + J_{e,p} \tag{3}$$

where the electron current density J_e is given mainly by J_{TF}; $J_{e,p}$ is the electron current density from plasma to the cathode, and J_i is the ion current density. The influence of the $J_{e,p}$ can be neglected and for the current density is obtained:

$$J_T = J_i + J_e \tag{4}$$

The total current density, from other hand, can be calculated as a ratio between the arc current I_a and cathode spot area $S_{cs} = \pi r_{cs}^2$, where r_{cs} is the cathode spot radius [1, 26].

$$J_T = \frac{I_a}{S_{cs}} \tag{5}$$

The electric field at the cathode E is calculated by equation [5, 9, 11]:

$$E^2 = \frac{4}{\varepsilon_0} J_T \left[(1-s)\sqrt{\frac{M}{2e}} - s\sqrt{\frac{m_e}{2e}}\right]\sqrt{V_C} \tag{6}$$

where: M is the ion mass, V_C is the cathode fall, s is the fraction of current carried by electrons in the cathode spot region; $J_T(1-s)$ is equal to the ion current density and $J_T s$ is equal to the electron current density, so the equation Eq.(6) can be writes as:

$$E^2 = \frac{4}{\varepsilon_0}\left[J_i\sqrt{\frac{M}{2e}} - J_e\sqrt{\frac{m_e}{2e}}\right]\sqrt{V_C} \tag{7}$$

The power density of heat conduction in the cathode body is estimated as is presented in [26]:

$$S_T = \frac{K_T(T_s - T_0)\sqrt{\pi}}{r_{cs}} \tag{8}$$

where: T_s is the cathode spot temperature, $T_0 = 300K$ is the temperature far from the cathode spot (the ambient temperature), K_T is the thermal conductivity of the cathode material.

The Joule heating power density, in a massive cathode, is calculated following the method of Rich [31] reduced to the cathode spot area:

$$S_J = \frac{32 r_{cs}}{100\sigma_{el}} J_T^2 \tag{9}$$

where σ_{el} is the electrical conductivity of the cathode material.

The energy balance at the cathode surface is expressed as [1]:

$$\frac{J_i}{e}(eV_c + V_i - \phi_{eff}) - \frac{J_e\phi_{eff}}{e} + \frac{2kT_e J_{e,p}}{e} - \left(W_{ev} + \frac{2kT_s}{m_n}\right)\Gamma_T m_n - \sigma_{sb}T_s^4 + S_r + S_J - S_T = 0 \tag{10}$$

where V_i is the ionization potential, S_r is the radiation from the plasma, W_{ev} is the energy of evaporation (J/kg), and σ_{sb} is the Stefan-Boltzmann constant. In the Eq. (10): the first term expresses ion impact heating; the second term expresses electron emission cooling; the third term expresses heating from the back-flux of plasma electrons; the fourth term expresses evaporative cooling; the fifth term expresses radiative cooling from the cathode surface; the sixth term expresses the plasma radiation; the seventh - expresses the Joule heating; and the eighth term expresses the conductive cooling. The third and the sixth term have an insignificant influence in the equation, so they can be neglected. Therefore the balance expression can be writes as:

$$\frac{J_i}{e}(eV_c + V_i - \phi_{eff}) - \frac{J_e\phi_{eff}}{e} - \left(W_{ev} + \frac{2kT_s}{m_n}\right)\Gamma_T m_n - \sigma_{sb}T_s^4 + S_J - S_T = 0 \quad (11)$$

By Eq. (11) is calculated full flow of particles which have left the cathode, including the particles forming cathode sheath plasma, irreversibly left the cathode particles, as well as those which are returned to the cathode. We are only interested in the cathode erosion - those particles that irreversibly cathode-out particles. The technical and the practical realizations of the PVD systems have influence on the cathode material evaporation processes. So, to be accounted this influence in the calculation procedure is included a correction factor. The correction factor is determined experimentally once-through for each type cathodes (first generation, second generation, and etc.). When the correction factor has determined, the erosion of the cathode material (Ti, Al, Cr, and etc.) is calculated for the respective cathode type.

CALCULATIONS

The presented mathematical model for prediction the erosion of the cathode material in PVD systems has follows steps: chosen value of the arc current; determination the cathode spot radius; calculation the total current density; calculation the ion and electron current density; calculation the electric field value; calculation the effective work function of the cathode material; calculation the cathode spot temperature; calculation the Joule heating; calculation the conductive cooling; and calculation the evaporated quantity material.

To illustrate the calculation procedure, an example of metal evaporation of massive cylindrical shape titanium cathodes in vacuum environment is used, as the arc current is chosen to be 70 A. The cathode spot radius is determined according the value of the arc current by the extrapolation of the Fig. 12 from [17]. For the chosen arc current the cathode spot radius is $r_{cs} = 4.6125 \times 10^{-6}$ m.

The total current density is calculated by the Eq.(5) and it is $J_T = 1.047 \times 10^{12}$ Am^{-2}. The ion current density for titanium cathode is 8% from the total current density [28,29], so the ion current density, for in the example, is $J_i = 8.378 \times 10^{10}$ Am^{-2}. Therefore using the Eq.(4) for the electron current density is received $J_e = 9.635 \times 10^{11}$ Am^{-2}.

The electric field value of $E = 9.248 \times 10^9$ V/m is calculated by the Eq.(7). The Joule heating is calculated by Eq.(9): $S_J = 6.8 \times 10^{11}$ Wm^{-2}. The conductive cooling $S_T = 2.394 \times 10^{10}$ Wm^{-2} is calculated by Eq.(8). So the full flow of evaporated particles of the material (the total heavy particle flux [1]) $\Gamma_T = 2.986 \times 10^{30}$ atoms/(sm^2) is calculated by Eq.(11), which is 57.58×10^{-3} kg/h for the 70A arc current.

Several measurements have been made on the used massive cylindrical shaped titanium cathodes, according to which the data for erosion rate is 9033 Ah/kg, which means that with the arc current of 70A the erosion rate is 7.75×10^{-3} kg/h, or 13.46% from the calculated value Γ_T is the real evaporated quantity of material. Therefore, the correction factor for the massive cylindrical shape cathode is 0.1346.

Fig. 1 shows the evaporation rate of the massive cylindrical shaped titanium cathode as a function of the arc current.

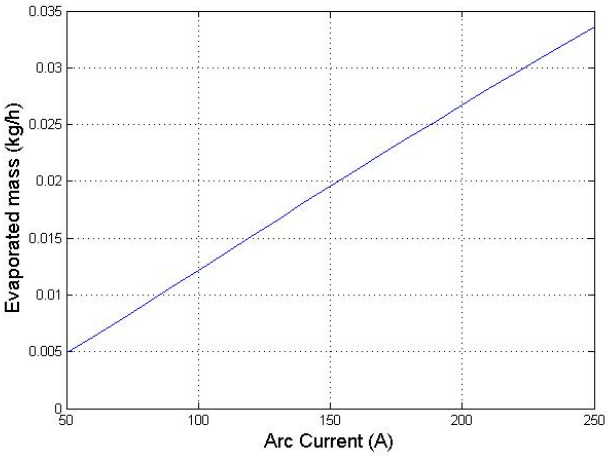

Fig. 1. The evaporation rate of the massive cylindrical shape titanium cathode as a function of the arc current.

CONCLUSIONS

Predicting the erosion of the cathode material in cathodic arc evaporation of metal in a vacuum environment is an interesting task with a variety of applications. The paper presents the model to predicting the erosion of the cathode material in PVD systems. The model gives the correlation between the arc current and the evaporated quantity of the cathode material in PVD processes. Additional preliminary information as the cathode spot temperature and/or the vapor pressure of the cathode material is not necessary.

Correction factor that represents the differences in technical terms of the metal evaporation process in vacuum environment by electric arc is introduced in the model. The correction factor is determined experimentally once-through for each generation cathodes. When the correction factor is determined, the erosion of different cathode material can be calculated.

The model has been developed on the basis of massive titanium cathodes and is applicable to all massive metal cathodes evaporated by an electric arc in vacuum environment by DC arc.

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ПРЕДСКАЗВАНЕ НА ЕРОЗИЯТА НА МАТЕРИАЛА НА КАТОДА ПРИ PVD СИСТЕМИ

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(Резюме)

Предсказването на ерозията на материала на катода при системите за катодно дъгово изпарение на метали във вакуумна среда е интересна задача с различни приложения. В този материал е представен метод за изчисление на изпареното количество вещество на материала на катода като функция от тока на електрическата дъга, чрез която той се изпарява. Методът е подходящ за процеси на катодно дъгово изпарение на метали във вакуумна среда на масивни катоди чрез постояннотокова дъга. Въведен е коригиращ коефициент, чрез който се отчитат различията в техническо отношение и при техническата реализация на самия процес на изпарение при различните PVD системи като геометрията на катода и магнитните му полета. Коригиращият коефициент се определя експериментално еднократно за всеки геометричен тип катоди. Методът е илюстриран чрез катодно дъгово изпарение на масивни цилиндрични катоди.

Възможността да може да се определя количеството изпарено вещество от катода в зависимост от големината на тока на дъгата, при системите за катодно дъгово изпарение на метали във вакуумна среда е решаващо, или е първа стъпка към моделирането на процесите на израстване на слоеве в този PVD системите.