

Modelling of process formation of the nanocomposite TiN-Cu layers received by vacuum-arc evaporation of Ti and magnetron sputtering of Cu

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Abstract. Modeling a TiN-Cu layers deposition process on a fused silica substrate under given conditions is carried out in this work. Calculation formulas which allow to determine the films thickness and their uniformity, with a substrate holder being located at an angle of 45 degrees to the normals of mutually perpendicular planes of the evaporated titanium cathode and the magnetron sputtering copper cathode, are given. The results of this work will be used to analyze the distribution velocity of the substance condensation flow and the character of the formed composite layers depending on the geometry of the cathode-substrate system.

1.Introduction

The studies connected with the development of new technologies for making composite layers with good plasticity and high hardness are of great interest. In this regard, creating composite coatings TiN-Cu by combining two discharge processes (vacuum arc evaporation of titanium in a nitrogen-containing plasma and ion-plasma sputtering of the copper target) is proposed. The design features of the installation realizing this approach, various forms of condensation surfaces, the heterogeneity of the streams density distribution and their characteristics in the working volume – they all put geometric factors in a number of insufficiently studied parameters significantly affecting the properties of the received coatings [1].

There are a number of reports [1-5] on calculating the parameters of a coating process (current density, deposition rate and the coating thickness) by the method of vacuum-arc evaporating or the method of magnetron sputtering at different points of a vacuum chamber. However, they are not suitable for calculations when the substrate holder is positioned at an angle of 45 degrees to the normals of the evaporated titanium cathode and the sputtering copper magnetron cathode planes perpendicular to one another. At the same time the properties of the obtained coatings are largely determined by the deposition rate and the character of their distribution on the condensing surface and the layer thickness.

This report is devoted to studying the condensation distribution speed of substance flows generated by a vacuum arc evaporator and a planar magnetron, the thickness of the obtained coatings and the character of the formed layers depending on the geometry of the cathode – substrate system.

2.Model description



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We will make a deposition process model for the case when the target and the substrate are not parallel, but are coaxial. In this case the sputtering angle and the angle of condensation are not equal, i.e. $\varphi \neq \phi$. Calculations of the film thickness were made according to the angle of condensation, and it was 45 degrees. At the same time we will make the following assumptions: I – the sprayed and evaporated atoms have a directional movement and are distributed in space according to the cosine law; II – the atomized and vaporized atoms do not collide with each other and with the atoms of the working gas, III – the sprayed and evaporated atoms are condensed at the point of impingement with the substrate.

In our calculations the expression for magnetron sputtering (2) was used. The expression (10) was used to determine the film's thickness in case of the flat disk evaporator sizes being final with the radius of R' .

The geometric scheme of the model «target -substrate» is shown in figure 1.

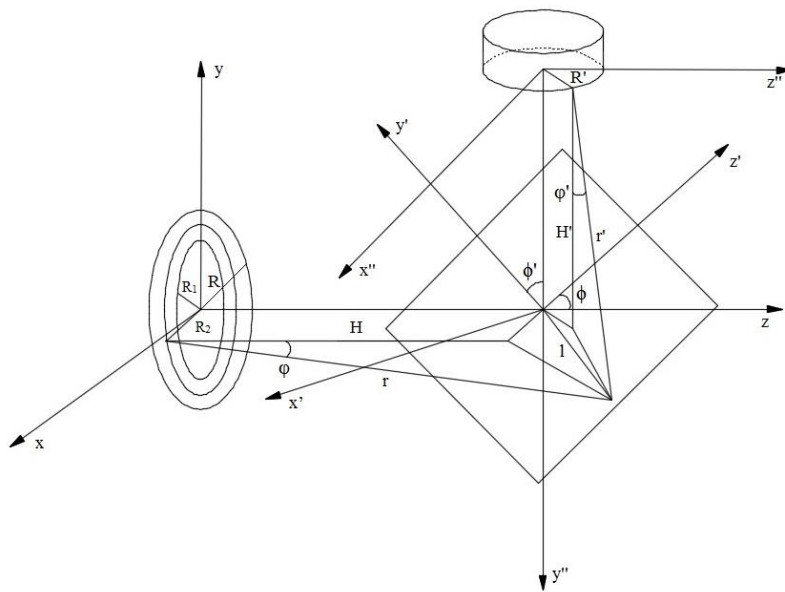


Figure 1. The geometric scheme of the model

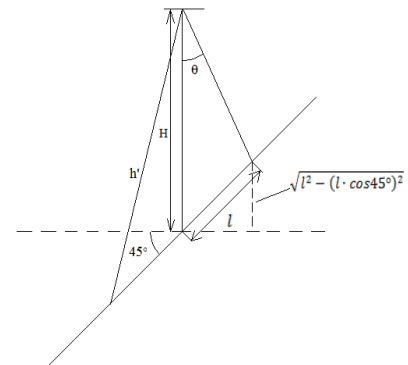


Figure 2. The geometric scheme of the distance changes between the cathode and the substrate

Method of a magnetron sputtering. In general, the thickness of the film at any point of the substrate is described by the expression:

$$h = \frac{V}{\pi \cdot r^2} \cos \varphi \cdot \cos \phi \cdot t \quad (1)$$

where V is the sputtering rate in thickness;

φ is the angle between the normal of the sputtering surface and the sputtering direction;

ϕ is the angle between the normal of the substrate's surface and the direction of deposition;

r is the distance between the sputtering element and the deposition point;

t is sputtering time.

We will use numerical integration of expression (2) in the calculations [6].

$$h = 2 \cdot V \cdot t \int_{R_1}^{R_2} \frac{H^2 \cdot R}{\left[(H^2 + R^2 - l^2)^2 + (2 \cdot l \cdot H)^2 \right]^{3/2}} dR \quad (2)$$

where H is the distance between the cathode face and the processed surface;

l is a coordinate along the surface of the substrate (the distance between the center of the substrate and a surface processed);

R is a cathode radius.

In figure 2 the change in the distance between the cathode and the substrate is schematically shown if the condensation angle is 45 degrees for magnetron sputtering and vacuum arc evaporating.

The distance H between the cathode end and the substrate element changes in accordance with expression (3), depending on the positive or negative values of l .

$$H' = H \pm \sqrt{l^2 - (l \cdot \cos 45^\circ)^2} \quad (3)$$

The sputtering rate is a quantitative characteristic of the materials ionic sputtering process which is defined as:

$$V = \frac{h}{t} \quad (4)$$

where h is the thickness of the sputtered material;

t is sputtering time.

It is possible to use the expression (4) for calculating the sputtering rate:

$$V_{sput} = \frac{j_i \cdot S \cdot M_a}{e \cdot N_a \cdot \rho} \quad (5)$$

where j_i is the ionic current density in the cross section perpendicular to the direction of falling ions;

S is a coefficient of material sputtering;

M_a is the atomic mass of the target atoms;

e is an elementary charge;

N_a is Avogadro's number;

ρ is the material density.

According to Sigmund's theory for amorphous and polycrystalline materials with the energy of ions less than 1 keV the sputtering coefficient is defined with the help of the following expression [6]:

$$S = \frac{3}{\pi^2} \alpha \frac{M_i \cdot M_a}{(M_i + M_a)^2} \cdot \frac{E_i}{2 \cdot E_{sub}} \quad (6)$$

where M_i and M_a are atomic masses of ions and atoms of the target;

E_i is falling ions energy;

E_{sub} is the sublimation energy of the target atoms [6];

α is a dimensionless parameter depending on the M_i/M_a .

The ionic current density is calculated according to the formula:

$$j_i = \frac{I}{S_r} \quad (7)$$

where j_i is the ionic current density in the cross section perpendicular to the direction of falling ions;

I is the discharge current;

S_r is the area of the sputtering ring. It is defined by the following expression:

$$S_k = \pi \cdot (R^2 - (R - b)^2) = \pi \cdot b(2R - b) \quad (8)$$

where, R is the sputtering radius;

b is the width of the sputtering ring;

Method of a vacuum-arc evaporation. When a sufficiently high negative potential is applied to the treated surface which is in plasma the ionic current of saturation is supplied to the surface. The magnitude of this ionic current in nonequilibrium plasma is given by the formula of Bom [7].

$$j_{H',l} = \frac{\mu_\rho \cdot I_a \cdot \bar{z}_i}{\pi \cdot m_i \cdot (R'^2 + H'^2)} \quad (9)$$

where μ_ρ is the coefficient of cathode erosion [10];

I_a is the arc current;

m_i is the mass of condensed ion;

R' is the cathode radius;

H' is the distance between the cathode end and the treatment surface;

\bar{z}_i is the average charging number of ions.

Depending on technological modes of the deposition process it is possible to calculate the ionic current density at an arbitrary point of the vacuum chamber by the formula [3]:

$$j_{H',l} = \frac{\mu_\rho \cdot I_a \cdot \bar{z}_i}{2\pi \cdot m_i \cdot R'^2} \left[1 + \frac{R'^2 - H'^2 - l^2}{\sqrt{(R'^2 + H'^2 + l^2)^2 - 4R'^2 \cdot l^2}} \right] \quad (10)$$

where l is a coordinate along the surface of the substrate (the distance from the center of the substrate to the treated surface).

According to figure 2 the distance H between the cathode end and the substrate element changes in accordance with expression (3), depending on the positive or negative values of l .

We will use the following expression to determine the coating layer thickness at an arbitrary point of a vacuum chamber:

$$h = V_c \cdot t \quad (11)$$

where V_c is the coating condensation rate;

t is the deposition time;

The coating condensation rate is defined from a ratio:

$$V_c = \frac{m_i}{z_i \cdot e \cdot \rho} \cdot \sum_{i=1}^n (\alpha_c \cdot j_{H',l} - S_{sp} \cdot j_{H',l}) \quad (12)$$

where ρ is the unit weight of the condensed substance;

α_c is the condensation coefficient;

S_{sp} is the sputtering coefficient.

While coatings being deposited, the substrate sputtering coefficient will aspire to zero, so it may be neglected. At the same time the condensation coefficient may be accepted equal to 1. Then the equation (12) will take the following form:

$$V_c = \frac{m_i \cdot \alpha_c \cdot i_{H',l}}{z_i \cdot e \cdot \rho} \quad (13)$$

3. Results and discussion

According to the model described above the calculation algorithms are realized in the software package Mathcad:

- layer thickness when the substrate holder is located at an angle of 45 degrees to the normals of the evaporated titanium cathode and sputtering copper magnetron cathode mutually perpendicular planes;
- the dependence of the deposited layer thickness on the offset relative to the cathode axis and the cathode-substrate distance, with the graph plotting (fig.3, 4).

We should say that the calculations were made for the separate work of the magnetron and vacuum-arc evaporator. Further the case of the evaporator and the magnetron simultaneous operation will be studied when the layer condensation will be fulfilled with two overlapping streams of the substance atoms.

The distribution of the deposited film thickness depending on the plate radius and distance to the cathode is the result of the calculations in the software package Mathcad. These distributions are shown on the following graphs:

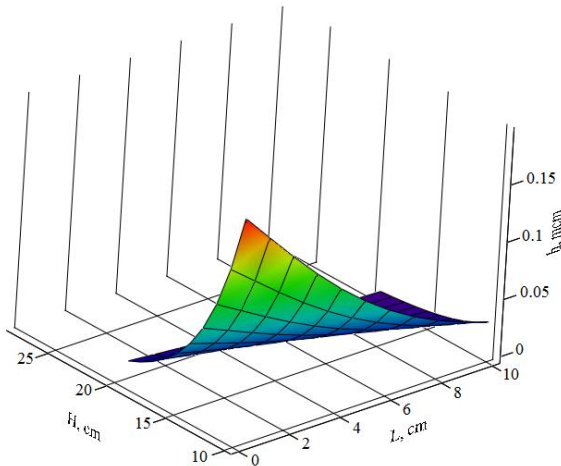


Figure 3. Distribution on thickness of a deposited layer from the offset relative to the cathode axis and distance to magnetron cathode

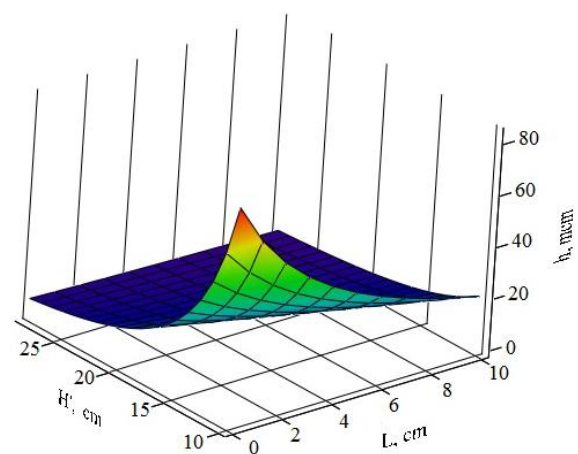


Figure 4. Distribution on thickness of a deposited layer from the offset relative to the cathode axis and distance to evaporator cathode

The calculation was carried out for coating deposition on the VU-1M installation. In Table 1 the process parameters, equipment characteristics and constants used in the calculations are shown.

Table 1. Values of the parameters and constants used in calculations

t, min	S (Cu), atom/ion	M _a (Cu), g/mol	e, C	N _a , atom/mol	ρ, g/cm ³	M _u , g/mol	α	E _{sub} , eV	L, cm
20	1,503	63,5	1,6x10 ⁻¹⁹	6,023x10 ²³	8,96	40	0,33	3,56	5
R, cm	I, A	H, cm	μ _p , kg/C	m _i , kg	z _i	α _k	R _k , cm	I _d , A	H', cm
6	4	10..19	53*10 ⁻⁹	79,5*10 ⁻²⁷	1,79	1	3	90	10..28

Experimental studies on deposition of layers by magnetron sputtering and vacuum arc evaporation have been conducted previously [8, 9]. In the case of vacuum-arc evaporation (H=28 cm L=0 cm) the layers thickness was 5-7 μm and in the case of magnetron sputtering (H=19 cm L=0 cm) it was 0.05-0.08 μm. The layer thickness depended on the deposition time t, arc current of evaporator I_∂, ion current density of magnetron I and the target material. The graphs show that the experimental data are in agreement with the calculated values for the vacuum arc evaporation. According to the figures one can see a significant effect of the geometric parameters of the cathode-substrate system on the uniformity of the coating thickness.

4. Conclusion

The method of calculating thicknesses of layers for separate processes of magnetron sputtering and vacuum arc evaporation in a plasma-chemical reactor is offered. Unlike the existing methods of calculation, this method takes into account the location of the substrate holder at an angle of 45

degrees to the normals of mutually perpendicular planes of a titanium evaporator cathode and a copper cathode of magnetron. Automated algorithms of calculating parameters and dependences of the layer thickness on the offset from the cathode axis and cathode-substrate distance have been carried out. This will allow to use the proposed calculation method to assess the film distribution uniformity along the radius of the substrate.

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