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EFFECT OF RE-EVAPORATION ON THE UNIFORMITY OF THE THICKNESS OF A FILM

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With complex kinematics characterizing the motion of the evaporator–substrate system, numerical modeling is used to study the effect of re-evaporation on the distribution of film thickness on the substrate.

The application of thin coatings by evaporation and condensation in a vacuum is usually done at pressures at which it is possible to ignore collisions among the molecules of the material being deposited and between these molecules and molecules of the residual gases. In such a free-molecular regime, the thickness of the film formed at point p of the substrate during the time τ is determined by the expression [1]:

$$d_P(\tau)=\frac{1}{\rho_I}\beta\frac{dm}{d\tau}\int_0^\tau\frac{\cos\varphi_P(t)\cos\psi_P(t)}{\pi r_P^2(t)}dt=\frac{1}{\rho_I}\beta\frac{dm}{d\tau}U_P, \quad (1)$$

where ϕ_p and ψ_p are the angles of evaporation and condensation; $dm/dt = S_I\rho_I c_I \exp(-M_I L_I/RT_I)$ is the rate of removal of material from the surface of the evaporator; R is the gas

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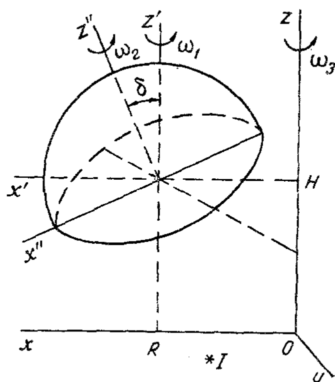

Fig. 1. Diagram of the vacuum deposition unit.

constant; C_I is the speed of sound in the material of the evaporator.

It should be noted that the evaporator, heated to high temperatures, is a source of radiation of appreciable intensity. In the free-molecular regime being considered, the flow of radiation from the evaporator is distributed in the same manner as the mass flow.

Conditions for the uniform distribution of the mass flows and the formation of a film of uniform thickness on surfaces have been studied for stationary surfaces [2], surfaces moving in the longitudinal direction [3], proper and planetary motion [1, 4], and a number of other cases. Here, the authors of [1-5] and other studies examined only the flow of mass from an evaporator.

In the present investigation, we study the formation of films with allowance for the reverse mass flow due to nonuniform thermal radiation from the evaporator.

Figure 1 presents a diagram of the motion of a spherical segment rotating about the axis of a chamber with the angular velocity ω_1 and about its own (natural) axis with the angular velocity ω_2 during vibrations of the natural axis relative to the chamber axis in accordance with the law $\delta = \delta_0 + A \sin \omega_3 t$. Here, δ is the running angle between the natural axis of the substrate and the chamber axis; δ_0 and A are the initial angle and amplitude of the vibrations; ω_3 is the angular velocity. The value of τ is determined as the complete period of the resulting motion of the system.

To analyze the process, we used a model based on the calculation of the motion of the unit normals of a coordinate system rigidly connected with a spherical segment in a stationary coordinate system [6]. The numerical calculations were performed with allowance for shielding of the molecular flow of the substance. Since analytical expressions were used at any moment of time to describe the position of the system and analyze the possibility of the substance ending up at point P on the substrate, the accuracy of the calculations is determined only by the time discretization.

Relation (1) is normally employed to calculate the thickness of a condensate deposited at a certain point of the surface [1, 3, 4]. However, the deposition process is usually accompanied by heating of the substrate and, thus, the origination of reverse flow of the substance due to re-evaporation. With allowance for the latter, the resulting mass flux at a given point of the surface is equal to

$$J = J_I - J_c, \tag{2}$$

where the mean mass flux from the evaporator during the period τ:

$$J_I = \frac{1}{\tau} \beta \frac{dm}{dt} U_P, \tag{3}$$

while the period-averaged flux of the re-evaporated material [7]:

$$J_c = \rho_I \left(\frac{RT_c}{2\pi M_I} \right)^{\frac{1}{2}} \exp\left(-\frac{M_I L_I}{RT_c} \right) \tag{4}$$

It should be noted that the time required to establish local thermal equilibrium during

deposition in a vacuum chamber [8] is only a small part of the total time of the process. This allows us to assume that the process takes place mainly with a steady-state temperature distribution on the substrate. This can be written in the form

$$T_c = \left[\frac{q_P}{\varepsilon\sigma} + T_w^4\right]^{\frac{1}{4}}, \tag{5}$$

where the period-averaged radiant flux from the evaporator to the substrate

$$q_P = \frac{1}{\tau}\varepsilon q U_P \tag{6}$$

is calculated in a manner similar to the mass flux; ε is the emissivity of the substrate; q is the radiant flux from the evaporator; σ is the Stefan–Boltzmann constant; T_w is the ambient temperature.

In accordance with (3) and (6), since the mass and radiation flows are proportional ($I_I \sim q_P$), the sections which receive more of the substance being deposited are heated more intensively and, in accordance with (4), re-evaporation takes place more intensively from these sections as well. Re-evaporation slows the growth of the condensate layer, this slowing occurring most intensively on the sections on which the greatest mass flux takes place. Thus, in a certain interval of rates, re-evaporation helps equalize the thickness of the layer over the surface. Re-evaporation is either absent or negligible at small values of q. At large values of q, re-evaporation leads to a situation whereby the reverse flux of material becomes equal to the forward flux. As a result, sections which are free of condensate appear on the surface.

It should be noted that the radiant flux density can be changed without changing its relative distribution on the substrate by the introduction of additional sources located in the plane of the evaporator. These sources are positioned symmetrically relative to the axis of the chamber.

Figure 2 shows results of calculations in which aluminum (L_I = 8.5 kJ/kg, M_I = 27, $\rho_I = 2.7 \cdot 10^3$ kg/m²) was chosen as the substance to be deposited. We used a plane evaporator of radius 10^{-2} m with the temperature T_I = 1400 K, $S_I = 3.14 \cdot 10^{-4}$ m².

As was noted above, the distribution of the thickness of the layer can be equalized by varying the radiant flux reaching the surface. However, the range of permissible values of q for these purposes is narrow. Thus, to deposit aluminum, the range of q which is effective for equalizing the thickness distribution lies within the interval 1-2 kW. As calculations showed, at $q < 1$ kW re-evaporation is either absent or has a negligible effect on the process. At levels of power greater than 1.3 kW, the flux J_c reaches the values of J_I, and condensate ceases to reach certain sections of the surface. The value of the upper boundary of q for effective equalizing evaporation depends appreciably on the incident flux J_I and its distribution on the surface, i.e. the temperature of the evaporator T_I, the distance of the substrate from the evaporator, and the kinematics of the system insofar as it determines the percentage of substance reaching at point on the surface. Also, with an increase in q, along with an increase in the uniformity of the distribution of the thickness of the condensate layer, there is a reduction in the thickness of the coating as a whole (the relation $d_f(q)$, Fig. 2). Here, d_f is the thickness of the film formed during one complete period of motion at the tip of the vertex of a spherical substrate. In other words, at $q \gtrsim 1.3$ kW, the deposition process becomes inefficient due to a reduction in its rate as a result of re-evaporation. The character and intensity of the reduction in d_f with an increase in q also depends on the kinematics of the process.

It should be noted that re-evaporation may lead to different results in this range of q, depending on the organization of the motion of the system. If the regime of motion and the mutual location of the evaporator and substrate are such as to result in a relatively small variation of thickness, then re-evaporation leads to additional equalization of the distribution $d_f(q)$ (lines 1 and 2 in Fig. 2a; lines 1-3 in Fig. 2b). Otherwise, re-evaporation does not lead to a significant increase in the uniformity of the coating (Fig. 2c and d). This is connected with the fact that the reverse flux J_c, connected with the incident radiant flux q_P through the temperature (4), depends nonlinearly on the incident flux J_I and thus cannot equalize the appreciable jumps in condensate distribution over the surface.

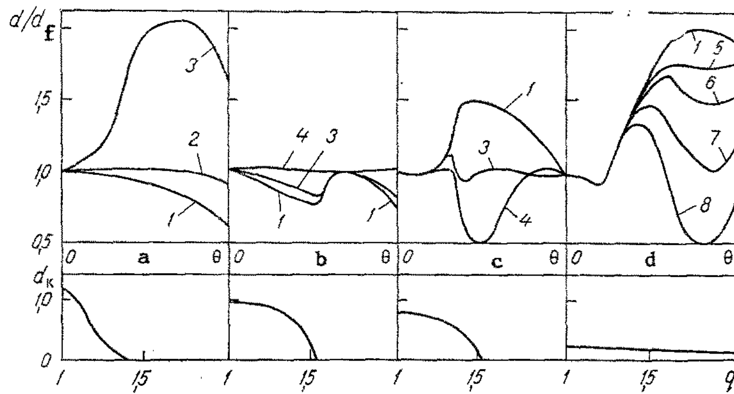

Fig. 2. Effect of re-evaporation on the distribution of the thickness of the condensate layer. The radius of the substrate r = 0.1 m, R = 0.2 m, H = 0.52 m, x_I = 0.18 m, y_I = 0, δ_0 = 45°, $w_1 = \pi$: 1) q = 1; 2) 1.1; 3) 1.2; 4) 1.3; 5) 1.4; 6) 1.5; 7) 1.6; 8) 1.7 kW: a) δ_0 = 50°, $w_{21} = w_2/w_1$ = 0.5, $w_{31} = w_3/w_1$ = 1; b) δ_0 = 60°, w_{21} = 2, w_{31} = 0.5; c) δ_0 = 70°, w_{21} = 0.5, w_{31} = 0; d) δ_0 = 80°, w_{21} = 2, w_{31} = o. d_f, μm; q, kW.

NOTATION

r_P, position vector of point P of a spherical segment; T_I, temperature of the evaporator; S_I, area of he evaporator; M_I, molecular weight of the substance being evaporated; L_I, heat of vaporization; ρ_I, density; β, adhesion coefficient.

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