STATISTICAL MODELING OF THE FILM-COATING PROCESS IN A VACUUM

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We describe the application of the method of statistical modeling through the use of an electronic digital computer to solve the problem of the distribution of film thickness for various geometric and physical parameters in the elements of a deposition system.

In depositing film in a vacuum one of the requirements imposed on the film is the fact that a specified distribution through the thickness must be achieved. The distribution of the film thickness depends strongly on the geometric shape and the mutual positioning of the elements of the chamber in which the deposition takes place. The distribution of the thickness is also affected by the distribution of the spatial flux of the molecules from the vaporized material and by the physical properties of the chamber surfaces (the molecular reflection coefficients, the law governing molecular reflection, etc.).

Below we demonstrate the possibility of calculating the distribution of the film thickness by the method of statistical modeling [1] through the use of an electronic digital computer. This method makes it possible to solve this problem for extremely broad hypotheses with respect to the geometry of the system and with respect to local laws governing the behavior of the vapor molecules at the surface.

The modeling algorithm and the program based on that algorithm for the M-20 computer are universal in the sense that they do not require change in carrying out the calculations for systems with various geometric and physical parameters of the elements.

1. Formulation of the Problem. We are considering a chamber (with an inside surface Q) for the deposition of films by vaporization of a substance in a vacuum. The chamber contains the source for the deposited substance, limited by surface F, and a receiver surface S (the backing). The geometric shape of the surfaces Q, F, and S, as well as their mutual positions, may be arbitrary, but are assumed to be specified.

Let the local physical laws governing the process of vapor–molecule transfer within the system be known:

1) the distribution $\sigma(M)$ for the rate of substance vaporization at the surface F of the source;

2) the reflection coefficients $R(M)$ for the vapor molecules at the surfaces of the system as functions of the point M at these surfaces;

3) the angular distributions $\gamma(M, \theta, \varphi)$ and $\omega(M, \theta, \varphi)$ in the space of the flux produced by the vapor molecule on vaporization and reflection.*

It is assumed that the vapor molecules move within the system without colliding with each other, nor with the molecules of the residual gases, and that they are moving at a constant velocity in all sections of the trajectory.†

* θ and φ are the polar and azimuthal angles in a spherical coordinate system.
†The last of these assumptions is not absolutely necessary. Consideration of the local change in velocity has virtually no effect on the algorithm.

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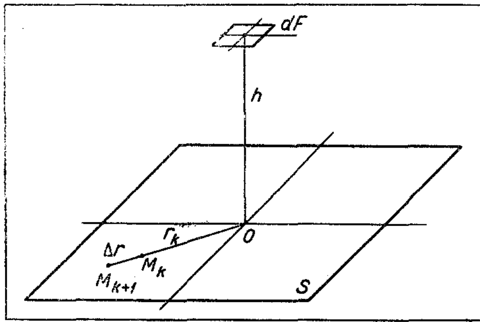

Fig. 1. Vaporization from a small area to a flat surface parallel to that area (h = 25 mm, Δr = 2.5 mm).

Under the cited assumptions with regard to the deposition process, we formulate the problem of calculating the film-thickness distribution δ(M) at the backing surface S on which a portion of the vaporized molecular flux is condensed after all of the possible multiple reflections from the surface of the system.

2. Method of the Solution for the Problem. The calculation of the distribution δ(M) is accomplished by the method of statistical modeling through the use of an electronic digital computer. We will give a statistical description for the application of this method to the film-coating process.

We will divide the backing surface S into n areas whose magnitude is chosen as a function of the required calculation accuracy. The film thickness at some point M_k of the surface of S will be approximately defined as

$$\delta(M_k) \approx \frac{\Delta m_k}{\rho \Delta S_k},$$

where Δm_k is the mass of the substance condensed in the area ΔS_k to which the M_k belongs; ρ denotes the density of the substance.

The mass Δm_k represents some portion of the mass m vaporized by the source. We can therefore write that $\Delta m_k = p_k m$, where p_k is some proportionality factor which corresponds to the area ΔS_k. Since the coating process is accomplished by the transfer of molecules (μ denotes the mass of molecules), we have $\Delta m_k = \mu N_k = p_k \mu N$, where N is the number of molecules released by the source, while N_k is the number of molecules condensed in the area ΔS_k. From this relationship we see that $p_k = N_k/N$, i.e., the factor p_k represents the frequency with which the molecules leaving the surface of the source reach the area ΔS_k and condense there.

Having calculated the values of the frequencies p_k for all of the areas ΔS_k, we can find the approximate distribution of the film thickness at the surface S, i.e.,

$$\delta_k = p_k \frac{m}{\rho \Delta S_k} \qquad (k = 1, 2, \ldots, n).$$

The algorithm for the calculation of the frequencies p_k is constructed directly from the given description of the deposition process. It is necessary to model the trajectories of a sufficiently large number N of molecules leaving the surface of the source, and to calculate the number of molecules N_k condensing in each of the areas ΔS_k (k = 1, 2, ..., n).

The calculation of the trajectories begins with the random position – in accordance with the distribution σ(M) – of the point from which the molecules leave the surface F. In accordance with the distribution γ(M, θ, φ) we randomly choose the direction in which the molecules move. We then determine the first rectilinear segment of the trajectory, for which we find the point P of molecular impact at one of the surfaces of the system [2]. In accordance with the physical properties of the surface, at the point of impact the molecule may either condense or be reflected. Examining the probability of molecular reflection at this point – equal to the reflection coefficient R(P) – we determine which of the two possible events is realized.

If the molecule impinges on the backing surface and condenses, we determine the number of the area to which the point of incidence belongs, and we add one to the counter for the molecules of this area. We then begin the calculation of the trajectory for the following molecule.

If the molecule has condensed at some other surface of the system, this fact is not recorded and we begin the simulation of the trajectory for the next molecule.

If the molecule is reflected from the surface, the following segment of the trajectory is constructed in accordance with the known law of reflection ω(M, θ, φ) and the tracking of the molecule is continued.

Having thus simulated the trajectories for N molecules, we calculate the values for the frequencies p_k and the distribution of the film thickness at the backing surface.

3. Calculations Illustrating the Accuracy of the Simulation. A program has been compiled for the M-20 digital computer on the basis of the above-described algorithm and certain calculations have been performed. We will present the results from the calculation of the film-thickness distribution for two cases of the source-backing system. In this case we have specially selected systems whose geometry makes it possible theoretically to achieve the required distributions. Comparison of the calculations with the theoretical gives some idea as to the accuracy of the proposed method. The molecular condensation coefficient at the surface of the backing was assumed to be equal to 1.

Example 1. Vaporization from a small area to a flat backing surface parallel to that area. It is assumed that the angular distribution of the molecules on vaporization from a small area is subject to the cosine law. We have theoretically derived [3] the formula for the ratio of the film thickness δ(M) at the point M to its thickness δ_0 at the point O for the source dF (see Fig. 1) and it has the form

$$\tau(M) = \frac{1}{\left[1 + \left(\frac{r}{h}\right)^2\right]^2}. \quad (1)$$

To calculate τ(M) by the method of statistical simulation we isolated a circle on the backing surface with its center at the point O and a radius of R = 50 mm, which was broken down into 20 anular areas by circles whose radii are equal to $k\Delta r$ ($k = 1, 2, \ldots, 20$). The cosine law for the release of molecules by the source was simulated by means of a random-number pick-up, these numbers uniformly distributed through the interval [0, 1]. The angular distribution of the flow of the generated molecules will be subject to the cosine law, if for the i-th molecule the discharge angles θ_i and φ_i are found from the relationships

$$\cos 2\theta_i = 1 - 2\eta_i, \quad \varphi_i = 2\pi\eta_i',$$

where η_i and η_i' are random numbers uniformly distributed through the interval [0, 1].

On the basis of the described algorithm we found the values of the frequencies p_k and the quantities

$$\tau_k = \frac{\delta_k}{\delta_1} = \frac{\Delta S_1}{p_1 \Delta S_k} p_k \qquad (k = 1, 2, \ldots, 20). \quad (2)$$

For comparison of the derived distribution (2) with the theoretical distribution (1) we assumed that the quantities τ_k correspond to the point $r_k = (2k - 1/2)\,\Delta r$, for which we calculated the theoretical values.

Table 1 shows the computer-calculated (N = 15,000) and theoretical values of τ_k.

Example 2. Vaporization from a point source to a flat backing surface. For a point source we assume an isotropic law of molecular release. The calculation of distribution (2) for this case proceeds in the same manner as in the previous case. The difference lies only in the fact that it is the isotropic molecular-release law that is being simulated, i.e.,

$$\cos\theta_i = 1 - 2\eta_i, \quad \varphi_i = 2\pi\eta_i'.$$

The theoretical formula [3] for τ(M) has the form

$$\tau(M) = \frac{1}{\left[1 + \left(\frac{r}{h}\right)^2\right]^{\frac{3}{2}}}. \quad (3)$$

Table 1 gives the computer-calculated (N = 10,000) and the theoretical values of τ_k for this case.

TABLE 1. Distribution of Relative Film Thickness

Point number	Example 1		Example 2		Point No.	Example 1		Example 2	
	τ_k calculated	τ_k theoretical	τ_k calculated	τ_k theoretical		τ_k calculated	τ_k theoretical	τ_k calculated	τ_k theoretical
1	1,000	1,000	1,000	1,000	11	0,226	0,226	0,341	0,328
2	0,966	0,957	0,976	0,967	12	0,187	0,185	0,303	0,283
3	0,903	0,887	0,908	0,913	13	0,154	0,152	0,246	0,244
4	0,806	0,794	0,835	0,841	14	0,126	0,126	0,209	0,210
5	0,694	0,692	0,750	0,758	15	0,106	0,104	0,184	0,183
6	0,593	0,589	0,672	0,673	16	0,086	0,086	0,155	0,159
7	0,495	0,494	0,583	0,589	17	0,072	0,072	0,145	0,139
8	0,411	0,410	0,510	0,512	18	0,060	0,061	0,126	0,122
9	0,346	0,337	0,442	0,442	19	0,053	0,051	0,106	0,107
10	0,282	0,276	0,394	0,381	20	0,045	0,043	0,082	0,095

NOTATION

$\sigma(M)$	is the distribution of the vaporization rate for the substance at the surface F of the source;
$R(M)$	is the coefficient of molecular reflection at the point M of the system's surface;
$\gamma(M, \Theta, \varphi)$ and $\omega(M, \Theta, \varphi)$	are the angular distributions within the space of the molecular flux on vaporization and reflection;
$\delta(M)$	is the thickness of the film at the point M of the backing S;
m	is the mass of the material vaporized by the source;
pk	is the frequency of the events which occur as the molecules impact and condense on an area ΔS_k of the backing;
$\tau(M)$	is the relative film thickness at the point M;
θ_i and φ_i	are the angles of relief for the i-th molecule;
N	is the number of tracked trajectories.

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