ADSORBED LAYERS IN THE INTERACTION OF A RAREFIED GAS FLOW WITH A DEEPLY COOLED OPTICAL SURFACE

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A method of direct modeling of adsorbed layers and estimation of the mean thickness of the cryodeposit is considered. The theoretical results are compared with experimental data.

The creation of deeply cooled astronomical telescopes and the need for their prolonged operation in the conditions of space entails taking account of the interaction of a rarefied gas flow with cryosurfaces, since the cryodeposite formed in the adsorption of gas particles at a mirror surface may considerably impair the mirror characteristics (for example, a cryodeposit thickness of 2-10 μm may lead to 10-100-fold deterioration [1]).

Consider the modeling of cryolayer growth, taking account of the real operating conditions of optical systems (neutral structureless particles with an energy of up to 10 eV and a numerical density of 10^{15}-10^{20} m^{-3}; elastic collision of the particles with the surface, with no excitation of electron degrees of freedom; surface temperature 10-20 K). In these circumstances, the interaction is determined by Van der Waals forces [2], i.e., there is physical adsorption, and the interaction of the gas particle with the moving optical surface may be regarded as a two-particle interaction – with one atom of the surface or with a previously adsorbed particle (adparticle) [3].

The lattice-gas model of a system of interacting particles is chosen to describe the cryodeposit structure: the adparticles lie at the vertices of elementary cells continuing the crystalline structure of the surface; the horizontal cell dimension a is assumed to be a multiple of the interatomic distance a_0 of the surface.

The interaction of adparticles in a multilayer lattice structure is described [4] by a Hamiltonian whose variation on incidence of the next gas particle at the surface at point (i, j) is equal to the increase in free energy of the system

$$\delta H = \sum_{<i,j>} \alpha_{<i,j>} \xi + \eta - E_{ng}, \tag{1}$$

where <i, j> is the set of nearest points, and

$$\alpha_{<i,j>} = \begin{cases} 1, & \text{the point is occupied by an adparticle;} \\ 0, & \text{the point is free.)} \end{cases}$$

Since the energy of Van der Waals interaction of two particles $\varepsilon(x) \sim x^{-6}$ [2], where x is the distance between the particles, it is sufficient to take the four closest points as <i, j>.

Considering the set of surface atoms and adparticles as a thermodynamic system with a temperature T_S equal to the temperature of the optical surface, which is maintained constant on account of heat extraction, the probability of adsorption is obtained [4]

$$W = \exp(-\delta H / kT_s). \tag{2}$$

In the process, actual adsorption occurs with probabiliy p, which is determined below.

Consideration of the combined motion of the incoming particle and the adparticle (oscillator) at the cryosurface requires quantum-mechanical description. In [3], the possibility of describing the motion of the incoming particle at low T_S independently of the oscillator, by means of the following equation, was noted

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$$X'' + \frac{2m_g}{\hbar^2}(E_g - U(y))X = 0, \tag{3}$$

where y is the distance to the adparticle which is closest to the normal; X is the wave function.

Suppose that U is a rectangular well with one infinite wall and another of height $\varepsilon \equiv \varepsilon(l)$ at a distance l from the first. If adsorption is understood to mean incidence of the incoming particle in the potential well, the probability of adsorption p is the probability of the incidence of a particle of energy E_g at a distance $y \le l$ from the adparticle of the previous layer calculated from Eq. (3) using the condition that X be continuously differentiable and the normalization condition.

If $E_g \le \varepsilon$, the adparticle will have an energy E_{ng} from a discrete set of K nonzero values; when $E_g > \varepsilon$, particle motion is infinite, and it is assumed to be diffusely reflected. The absence of adsorption when $E_g > \varepsilon$ is confirmed by the experimental finding [5] that a particle may be captured if its energy is no greater than some characteristic value for the given surface and the form of gas particles.

Formalizing the direct-modeling process for a rectangular fragment of surface consisting of N•M points which are a distance a apart, the cryodeposit is represented as N•M columns of height h_{ij} at these points. The adsorption of a particle at the point (i, j) leads to increase in h_{ij} by ℓ, and desorption to decrease in h_{ij} by 2ℓ (the desporption condition is $E_n + E_g - E_{ng} > \varepsilon$, where E_n is the energy of an adparticle of the previous layer). The value of a is established from the condition of practical occurrence of adsorption $W \ge 0.05$, and from the condition $K > 0$.

Direct modeling begins with the calculation of the discretization interval τ of arrival of the incoming particles at the surface and the mean adsorption probability p. The column (k, j) is chosen randomly, as is the random Maxwellian velocity of the particle under the condition $E_g \le \varepsilon$; random realizations of the adsorption process are undertaken with probability W according to Eq. (2), where δH is calculated from Eq. (1) for the actual set of adparticles at points ⟨i, j⟩, and a probability of actual adsorption, if it occurs, of p. A discrete level E_{ng} is chosen, and the desorption condition is tested.

To accelerate the modeling, equiprobable classes of hypothetical and real interactions are introduced. On incidence in a class of hypothetical interactions, the experiment time is increased without modeling by an amount easily estimated from the mean probability of adsorption.

The new aspect of this method of estimating the thickness and rate of growth of the cryodeposit is associated with taking specific account of the features of low-temperature physical adsorption and the simplicity of the modeling procedure on account of the consideration of the spatially one-dimensional independent motion of the incoming particle and the introduction of a lattice structure of the cryodeposit. The validity of these simplifications is confirmed by comparing the calculation results with experimental data.

The interaction of atomic oxygen with a particle energy of ~5 eV and a Be surface at $T_s = 4.5$ K, $v = 8 \cdot 10^3$ m/sec, $n_g = 10^{15}$ m^{-3} is modeled. The values adopted in the calculation are: $a = 0.91 \cdot 10^{-9}$ m; $\ell = 0.54 \cdot 10^{-9}$ m; $p = 0.968$. It was noted in [1] that, in analogous conditions, a cryodeposit of thickness 1 μm was obtained experimentally in two weeks. The theoretical estimate is a thickness of 0.23 μm, which may be regarded as acceptable, since no direct statement of the value of n_g was given in [1] and it was chosen on the basis of the data of [6].

The interaction of oxygen and argon with an aluminum surface is modeled and the rate of increase in thickness of the cryodeposit V_g as a function of T_s is compared with the experimental conditions are: $T_g = 300$ K; $n_g = 3.2 \cdot 10^{18}$ m^{-3}; $v = 0$. As shown by the theoretical values of V_g in Table 1, the mean relative error in the given temperature interval is ~40%, which is acceptable in obtaining lower bounds on the operating period.

The results obtained confirm the practical utility of the algorithm proposed for modeling the gas absorption at optical cryosurfaces and estimating the growth rate of the cryodeposit, which permits the evaluation of the dynamics of possible cryodeposit growth in the actual operation of optical systems and the need for protection from contamination even at the stage of designing the system, as well as providing the basis for optimal stand test conditions.

TABLE 1. Theoretical Values of V_g as a Function of T_s

T_s, K	V_g, μm/min	
	oxygen	argon
10	0,090	0,124
15/13,5	0,197	0,127
20	0,275	0,147
30	0,370	0,156

Notation. T_s, surface temperature, K; a_0, interatomic distance, m; v, velocity of surface motion, $m \cdot sec^{-1}$; T_g, gas temperature, K; m_g, mass of gas particles, kg; a, ℓ, linear cell dimensions of lattice structure, m; U, interaction potential, J; ξ, interaction energy in layer, J; η, interaction energy of adparticles with closest adparticle in the next layer, J; ε, depth of potential well, J; δH, variation in free energy, J; W, p, probability of the process and fact of adsorption; N, M, number of points over the length and width of the fragment; h, Planck's constant; k, Boltzmann constant.

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