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Numerical investigation of rarefied gas atoms scattering from rough solid surface

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THE NUMERICAL algorithm of determination of the velocity distribution function for particles reflected from real rough surface is described. The rough surface geometry is determined by the analytical many-parametrical function with parameters, received from experimental study of the surface roughness. The distribution function of reflected particles is presented by means of three-dimensional diagrams. The method of computation is illustrated on several examples and may be applied in space investigations.

W pracy opisany jest numeryczny algorytm określenia funkcji rozkładu prędkości cząstek odbitych od rzeczywistych szorstkich powierzchni. Geometrię szorstkiej powierzchni określono za pomocą wieloparametrowej funkcji analitycznej, przy czym parametry zostały otrzymane z badań doświadczalnych szorstkości powierzchni. Funkcja rozkładu odbitych cząstek przedstawiona jest w postaci trójwymiarowych wykresów. Metoda obliczeń jest zilustrowana licznymi przykładami i może mieć zastosowanie w badaniach przestrzeni kosmicznej.

В работе описан численный алгоритм для определения функции распределения скоростей молекул, отраженных от реальных шероховатых поверхностей. Геометрия шероховатой поверхности определена с помощью многопараметрической аналитической функции, причем параметры получены из экспериментальных исследований шероховатости поверхности. Функция распределения отраженных молекул представлена в виде трехмерных графиков. Метод вычислений иллюстрируется многими примерами и может иметь применение в исследованиях космического пространства.

THE FLIGHT of convex bodies through the highly rarefied gas of the upper atmosphere proceeds under conditions of free-molecule flow, during which the flow past a fragment of the surface is independent of the flow past a neighbouring fragment, so that the computation of aerodynamic characteristics reduces to surface integration of the impulse of the incident and reflected molecules, acting on a surface element dS.

In works concerned with aerodynamical problems the surface is usually considered to be smooth [1] and the character of the reflection of molecules may be described by conventional mathematical laws (the cosine law, for instance). However, such an approach to the problem does not always, if high accuracy of computation of the aerodynamic characteristics is needed, satisfy the design requirements.

The surface of a real body is always rough, so that incident molecules collide with fragments of the surface having various locations with reference to a certain mean smooth surface. Elements dS of the surface may be considered to be smooth. Under conditions of great roughness, multiple collisions of a molecule with the surface are possible.

The research into problems of interaction between atoms and a rough surface was hitherto reduced, in principle, to a mathematical description of a rough surface and to the establishment of an impact transform [2] or to the numerical computation of the characteristics of the reflected flow in function of the roughness constants [3]. Practically no data are available on particular materials of which AES[1] structures are made.

In the present paper, we shall consider the interaction between gas atoms and a real rough surface. A method for determining the interaction parameters will be discussed. This method includes the known computation procedure for interaction parameters with a smooth surface [4].

For experimental determination of the roughness parameters of the surface, the measurement is, as a rule, performed in a certain plane section. If the surface is isotropic, the direction of the measurements is of no importance and the roughness profiles will be the same in any directions. If the measurement path is sufficiently long, we may consider the profile of the real surface to be approximately a stationary random function and apply harmonic analysis for the representation of the irregularity parameters.

The profile of a surface over a length l of measurement may be represented in the form of the Fourier series:

$$z(x) = A_0 + \sum_{i=1}^{n} R_i \sin(\omega_i x + \varphi_i), \tag{1}$$

where A_0 is the initial amplitude (which is constant), R_i — the amplitude of the i-th harmonic, $\omega_i = 2\pi/T_i$ — frequency, T_i — period and φ_i — phase angle. The symbol i denotes the number of dominant harmonics. All the components involved in this expression are determined by the profilogrammetric method of measurement of the roughness parameters.

The completeness of the representation of the profile by its harmonic components obtained as a result of this analysis is appraised by the ratio $R = \sum_{i=1}^{n} R_i^2/2H$, where H is the mean square deviation of profile points from the mean line. The degree of roughness of the profile is determined by the fluctuation of the slopes of the irregularities of the surface:

$$\sigma_1 = \sqrt{\sum_{i=1}^{n} (R_i\omega_i/2)^2/(n-1)}.$$

Thus, for instance, the parameters R and σ_1 for the surface of a chemically polished aluminium alloy have values of 0.69 and 0.0179, and for an anodized aluminium alloy — 0.86 and 0.02220, respectively — that is, the deflections R_i are nearer the mean square deviation for a rougher surface.

In general, the profile of a surface can be represented by any periodic analytic function. In particular, the transverse profile of glass fabric made of a yarn composed of thin cylindrical threads of uniform diameter is modelled by packed orthogonal cylindrical segments — that is, by the set of equations:

$$\begin{gathered} (x-r)^2+z^2 = r^2, \\ (x-3r)^2+z^2 = r^2, \\ \cdots\cdots\cdots\cdots\cdots \\ [x-(2n-1)r]^2+z^2 = r^2, \end{gathered} \tag{2}$$

where the radius of the thread is $r \approx 4\mu$.

[1] AES — Artificial Earth Satellite.

Since the roughness profiles of most materials obtained by measurement are constant for any azimuthal angle of the measurement path, it will be assumed in what follows that the gas interacts with a rough plane profile — that is, the problem of interaction is considered to be a plane problem until the impact of the gas particle on an elementary profile segment. From this moment on, the problem is three-dimensional. The impact of a particle proceeds according to the scheme of interaction with a smooth surface of a block of effective interaction and the particle reflected in any direction in the space. In the plane of reflection, which is determined by the element normal to the surface and the velocity vector of reflection, we are concerned with a plane profile, for which we can consider a second impact of the particle already reflected. This impact problem is again three-dimensional and so on, until the reflection (or capture) is complete.

Thus, in a small region, the impact of any particle is a collision with a smooth surface, the roughness consisting in the fact that the incidence angle at various points of the profile is different from the angle of attack (which is to be determined) and that multiple collisions of a particle with the surface are possible.

For a profile segment of length l, the coordinate x is selected at random and the relevant vertical coordinate $z(x)$ is found from the analytic representation (1) of the profile. Then, by finding the derivative, we determine the slope of the profile segment under consideration with reference to the mean smooth profile and find, for a known angle of attack, the real angle of incidence. By performing many times ($\sim 10^3$ to 10^4) the random selection of the coordinate x, the angles of slope can be grouped for this coordinate about a number of discrete values, of order 10 to 10^2, thus reducing the number of the trajectories for the determination of the state of incidence. Further analysis is the same as for a smooth surface.

When the atom of gas has been reflected from the surface element — that is, it has entered the zone of free motion, the condition of intersection of the trajectory (now rectilinear) of the rebounded atom with the profile curve $z(x)$ in the plane of reflection is verified. If there is intersection, we are concerned with a second collision. If not, the atom is considered to have been reflected, and all its characteristics are calculated by the method for a smooth surface.

If the profile is prescribed by the set of equations (2), the solution involves an additional parameter — the number n of the equations. The slope of the surface at a point selected at random depends on n and is given, for arbitrary n, by the equation

$$\frac{dz}{dx} = \frac{(2n-1)r-x}{z}$$

and the vertical coordinate is

$$z = \sqrt{r^2-[x-(2n-1)r]^2}.$$

It suffices to take a length $4r$ $(r, 5r)$ of the measurement path; therefore, the parameter n may become $1, 2, 3$, and is determined in an unequivocal manner for a coordinate x selected for that segment at random.

Computation shows that the probability of multiple collisions of reflected particles is small. Thus, independently of the form of (1) or (2) of the rougness profile, the probability of a third collision is practically zero, the probability of a second collision for a profile

(2) approaching 0.15, and being by one order of magnitude smaller for (1). It is obvious that the probability of multiple collision varies with varying roughness parameters R, σ_1, r.

As a result of calculation according to the above scheme, the following parameters of aerodynamic interaction between flowing gas and a rough surface are obtained: the angular velocity distribution v' of the rebounded particles over the surface — the ratio of the mean velocity of particles reflected in a direction determined by the angle of reflected ϑ' and the azimuthal angle of rebound φ' to the velocity v of particles of the onflowing stream, ϱ' — the angular distribution of density of reflected particles above the surface — the ratio of the number of particles rebounded in the direction determined by the angles ϑ' and φ' with a velocity v', to the total number of incident particles; α_e, α_n, α_τ — the coefficients of accommodation of energy of the normal and tangential impulse. The values of the coefficients of accommodation are determined by averaging the results of computation for all the trajectories of the reflected particles (all the particles, colliding with the surface for a fixed angle of attack).

The scheme of reflection of molecules from a surface element is shown in Fig. 1.

Figure 2 shows the variation of the coefficients of accommodation of energy α_e and normal and tangential impulse α_n and α_τ, respectively, in function of the angle of in-

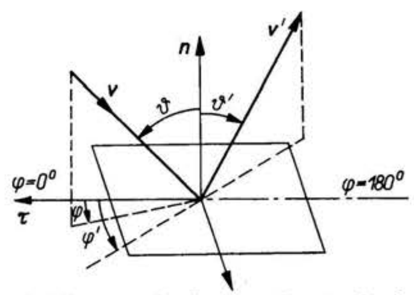

FIG. 1. Diagram of reflection of molecules from a surface element.

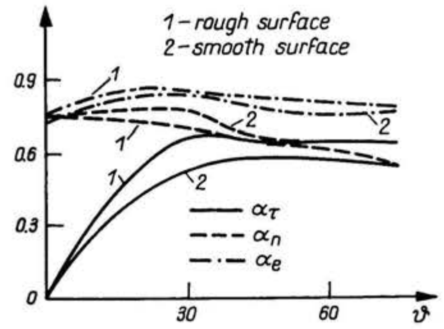

FIG. 2. Dependence of the accomodation coefficients on the incidence angle for the interaction between oxygen atoms and a chemically polished surface of an aluminium alloy ——— α_τ — — — — α_n, — · — · — α_e 1 – rough surface, 2 – smooth surface.

cidence of oxygen atoms on a chemically polished surface of an aluminium alloy. The number 1 concerns curves, obtained by taking into account the real roughness of the surface, and the number 2 — curves, for which the roughness is disregarded. It is easy to see that the influence of the roughness on integral characteristics, such as the coefficients of accommodation, is not very strong. Let us observe also that the roughness shows a still weaker influence on the drag coefficient, the maximum being 5%. The influence of the roughness on quantities, the obtainment of which is connected with less averaging, is both qualitative and quantitative.

Figures 3 to 5 show, by way of example, some selected numerical data for two gases (O and N_2) and three rough materials (aluminium alloy chemically polished or anodized and glass fabric). Figure 3 shows the velocity distribution of reflected particles with respect to the angle ϑ for some fixed rebound planes and a fixed incidence angle ϑ. For $\vartheta = 0°$ the curves of distribution are symmetric. In all the cases the diagram of reflection is symmetric about the plane determined by the vectors v and n.

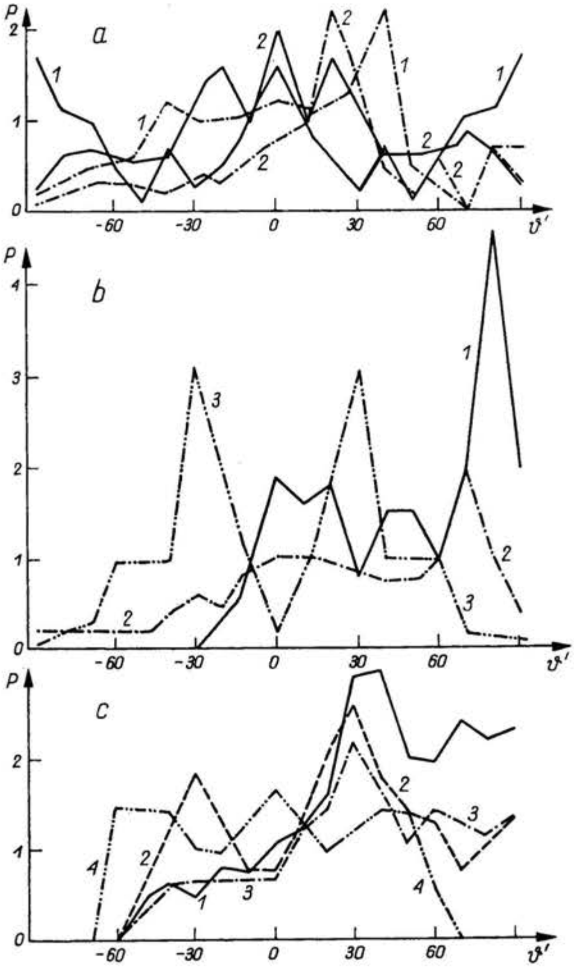

FIG. 3. Angular distribution of velocity of reflected particles —— $\vartheta = 0°$, — · — · —, — — —, — · · —, — × — $\vartheta = 30°$; $1 - \varphi = 0°, 180°$; $2 - \varphi = 30°, 150°$; $3 - \varphi = 60°\ 120°$; $4 - \varphi = 90°$; a) O – chemically polished aluminium alloy; b) N_2 – glass fabric; c) N_2 – anodized aluminium alloy.

The curves in Fig. 4 represent the function $\varrho'(v')$, which is the distribution function of reflected particles with respect to the direction and velocity. These distributions are normed, the density ϱ and the velocity v of incident particles being assumed to be units. Note that the curves have more than one peak for almost all the gas surface combinations.

The values of the impulse of reflected particles P, acting per unit area of the surface and computed according to the formula

$$P = \varrho' v' M \varrho v^2 S_1 M_1$$

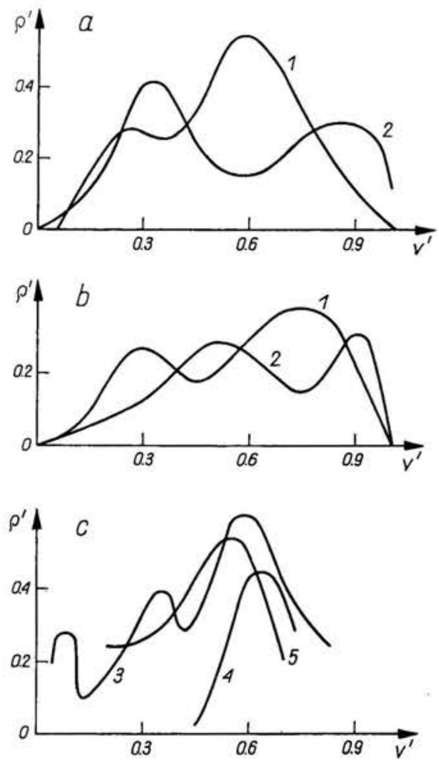

FIG. 4. Density of distribution of reflected particles according to the velocity in the plane $\varphi = 0°, 180°$; $1-\vartheta = 0°$; $2-\vartheta = 15°$; $3-\vartheta = 30°$; $4-\vartheta = 60°$; $5-\vartheta = 75°$; a) O – chemically polished aluminium alloy; b) N_2 – glass fabric, c) N_2 – anodized aluminium alloy.

in function of the incidence angle ϑ and the azimuthal angle of reflection φ' are shown in Fig. 5. The symbols in the formula above are as follows: ϱ — concentration of the gas component in the upper atmosphere at the flight altitude of the AES, S_1 — the area of the surface, M — the molecular weight of the gas component in hydrogen units, M_1 — the atom unit of mass.

For the determination of the influence of the surface roughness on the value of the coefficients of normal and tangential force component, P_n and P, respectively, acting per unit area of the surface, their values for a smooth and rough surface (the values of α_n, α_τ^1, α_e having been taken into account) have been determined according to the formulae

$$\frac{P_n}{q} = \Big\{(2-\alpha_n)\frac{\sin\alpha}{S\sqrt{\pi}}\exp(-S^2\sin^2\alpha)+(2-\alpha_n)\,(\sin^2\alpha+1/2S^2)\,[1+\mathrm{erf}(S\sin\alpha)]$$

$$+L/2S^2\sqrt{T_S/T}\exp(-S^2\sin^2\alpha)+\alpha_n\sqrt{\pi}\sin\alpha/2S\sqrt{T_S/T}[1+\mathrm{erf}(S\sin\alpha)]\Big\},$$

$$\frac{P_\tau}{q} = \alpha_\tau\frac{\cos\alpha}{S\sqrt{\pi}}\exp(-S^2\sin^2\alpha)+\alpha_\tau\sin\alpha\cos\alpha[1+\mathrm{erf}(S\sin\alpha)],$$

where $\alpha = \pi/2-\vartheta$ is the angle of attack, S — the ratio of the most probable thermal velocity of molecules of the onflowing stream to the average mass velocity of flow,

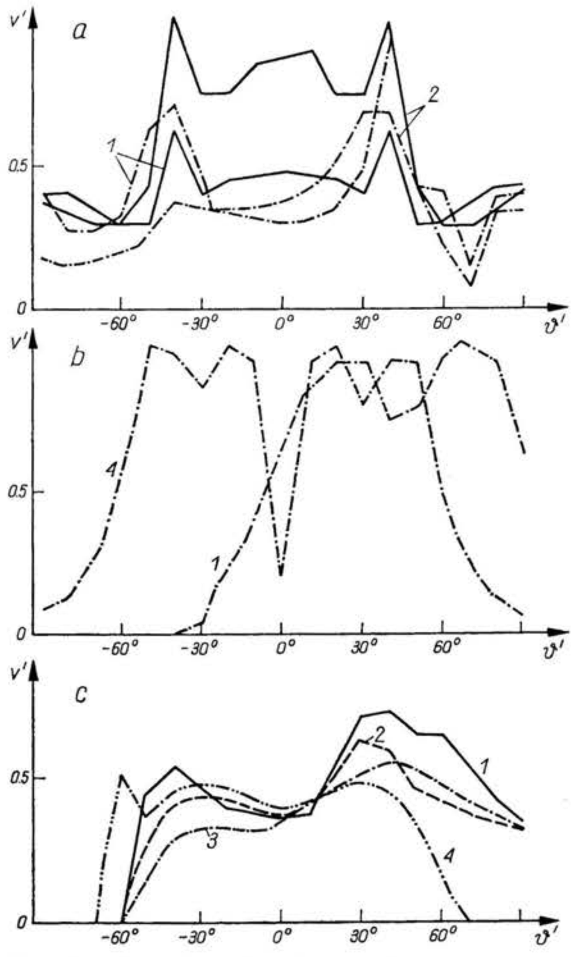

FIG. 5. Distribution of impulse of particles reflected from unit area of a rough surface; —— $\vartheta = 0°$; —·—·—, — — —, —··—, —×— $\vartheta = 30°$; $1-\varphi = 0°$; $180°$; $2-\varphi = 30°$, $150°$; $3-\varphi = 60°$, $120°$; $4-\varphi = 90°$, a) O – chemically polished aluminium alloy, b) N – glass fabric, c) N_2 – anodized aluminium alloy.

T — the temperature of the flowing gas, T_s — surface temperature of the AES and $q = \varrho v^2/2$ — aerodynamic velocity force.

The values assumed for the computation of P_n and P_τ were $S = 10$; $T = 1200°$, $T_s = 300°K$. They characterize the average flow conditions past the satellite at an altitude of about 200 km.

Figure 6 shows the values of P_n and P_τ for angles of attack within the interval from 0° to 90°, for the combination O — chemically polished aluminium alloy. The same figure shows, for comparison, the curves of P_n and P_τ, for $\alpha_n = \alpha_\tau = 1$.

From the numerical results it can be inferred that the number of particles reflected from a rough surface is smaller than the number of particles reflected from a smooth surface, more incident particles being captured by a rough surface, for which the accom-

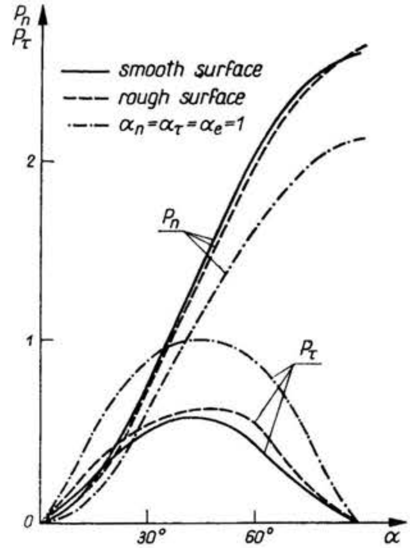

FIG. 6. Dependence of P_n and P_τ on the angle of attack for the combination O – chemically polished aluminium alloy; ——— smooth surface; — — — — rough surface; — · — · — $\alpha_n = \alpha_\tau = \alpha_e = 1$.

modation coefficients assumed to be units. As a result of this effect the value of the accommodation coefficients for a rough surface is, on the average, 5% higher than for a smooth surface.

Computation has shown that the characteristics of interaction as considered in terms of the distribution function are strongly influenced by the surface roughness. As the characteristics of interaction are found (for the computation of which averaging was performed in various variables), the influence of the surface roughness on these characteristics becomes smaller. However, even a rough appraisal shows that the surface roughness must be taken into account at every stage of averaging, the obtainment of the coefficient of aerodynamic drag C_d being included. It will be obvious that for different skin materials, various atoms of the onflowing gas and various degrees of roughness, the influence of the roughness on the parameters of aerodynamic interaction will be different.

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