Archives of Mechanics • Archiwum Mechaniki Stosowanej • 25, 2, pp. 253–258, Warszawa 1973

Computer study of gas atoms scattering from a solid surface with application to space problems

A. A. PYARNPUU (MOSCOW)

THE NUMERICAL algorithm of determination of the accomodation coefficients and the velocity distribution function for particles reflected from several crystalic surfaces is described. All main interaction parameters, the characteristics of incident flow and the properties of surface which may be presented by multicomponent alloy, are taken into consideration. The method of computation is illustrated on several examples and may be used in space applications.

Opisano algorytm numeryczny określenia współczynników przystosowania i funkcji rozkładu prędkości dla odbitych cząsteczek od kilku krystalicznych powierzchni. Rozważono wszystkie główne parametry oddziaływania, charakterystyki przepływu i własności powierzchni, które mogą wystąpić dla wieloskładnikowych stopów. Metoda obliczenia została zilustrowana na kilku przykładach i może być zastosowana w zagadnieniach przestrzeni kosmicznej.

Описан численный алгоритм для определения коэффициентов аккомодации и функции распределения скоростей частиц, отраженных от различных кристаллических поверхностей. Рассмотрены все основные параметры, характеристики набегающего потока, а также свойства поверхности многокомпонентного сплава. Метод вычислений иллюстрируется на нескольких примерах; его можно применить в задачах космической техники.

NUMERICAL experimental methods of studying the scattering of atoms from oriented surface elements of solids are on the whole well developed [1, 2, 3]. Consideration of the absorbed layer does not in principle involve any difficulties [2]. The dependence is studied of the distribution function for reflected particles and momentum and energy accommodation coefficients on initial parameter ϑ — the angle of incidence of the incident molecular beam on the surface element.

Taking into account the fact that the papers referred to pursued a single object — namely, the application of the accommodation coefficients obtained to the calculation of satellite drag at very high altitude, the replacement of real gas flow by the monoenergetic beam is a highly accurate approximation [1]. However, the satellite surface, although smooth in the technological sense (especially the surface of solar batteries, which form the basic part of the whole surface), will be rough on the molecular-crystalline level in which the approximate calculation is performed. Nevertheless, the assumption that the reflection of any molecule from the surface of the satellite takes place from some crystallographic facet of the surface material seems justified. Thus the dependence of the reflected flow parameters on the incidence angle ϑ is important because different elements of the satellite surface are oriented variously with reference to the incident flow, and there is a possibility

of approximate consideration of effects roughness on the interaction. In this paper, the last factor is disregarded.

The assumption usually made that the crystal of the solid is composed of a single molecular element simplifies the logic of the program and shortens the time by the computer for calculation. Actually, the surface material may not contain atoms of a single kind; as a rule, it contains alloys of two or more elements.

In this paper are presented the results of numerical computations of momentum and energy accommodation coefficients and angular distribution of energy of reflected particles. The surface was of crystallic structure, its type and internal connections depending on the kind of solid used. The gas molecule (N_2, Ar) interacts with a three-dimensional finite-size surface block consisting of Si, Ag, Fe, Ni, Cr, Al and Cu atoms, which may be contained in the crystal as alloys.

The computer program on ALGOL-60 for modelling of gas-surface interaction is worked out and the calculations are realized on the computer BESM-6. All the integral characteristics of interaction are calculated by averaging the results for individual trajectories of gas atoms according to method given in [1].

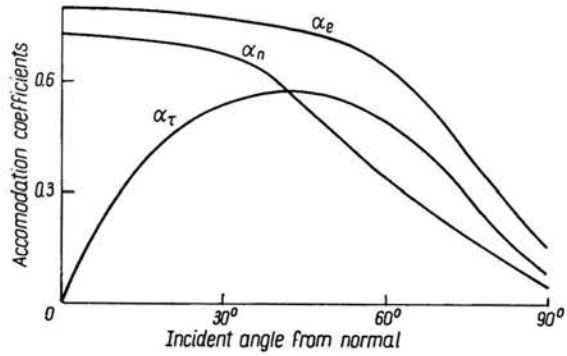

FIG. 1. Accommodation coefficients (N_2–Si, α_e—energy, α_n—normal momentum, α_τ — angential).

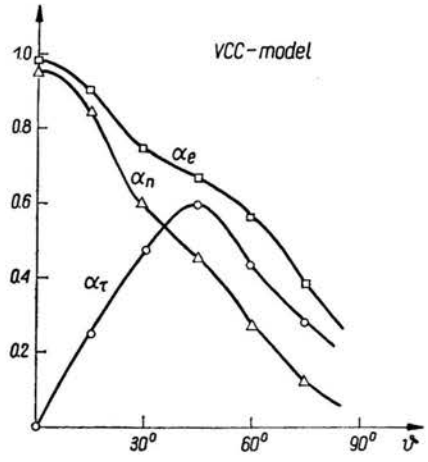

FIG. 2. Accommodation coefficients ($\mu = 0.1$).

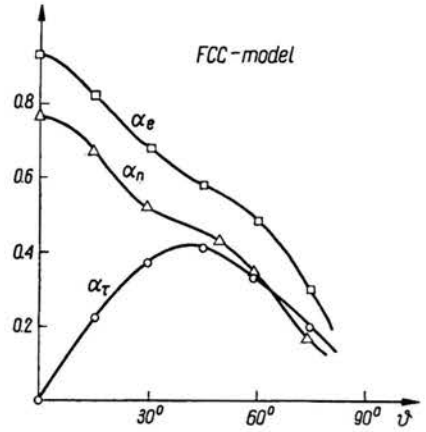

Fig. 3. Accommodation coefficients ($\mu = 0.1$).

Figure 1 shows the dependence of energy α_e, normal α_n, and tangential α_τ momentum accommodation coefficients on the incidence angle ϑ for nitrogen molecules on a silicon surface. The silicon crystal was of diamond structure; for purposes of comparison, in Figs. 2 and 3 are shown curves for volume centered (*VCC*) and face centered (*FCC*) cubic lattices. The lesser smoothness of these curves as compared to Fig. 1 is an effect of the lower density of *VCC* and *FCC* lattices. The effect of roughness increases also with reduction of the ratio of the mass of the gas molecule to the mass of the crystal atom, μ (in Figs. 2

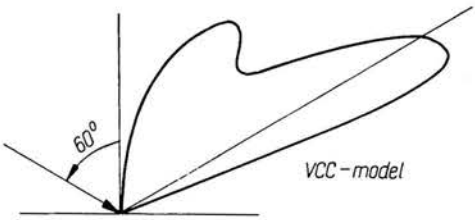

FIG. 4. Angular distribution ($\mu = 0.1$).

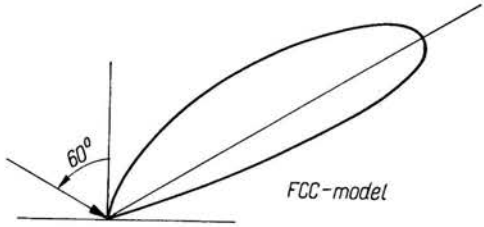

FIG. 5. Angular distribution ($\mu = 0.1$).

and 3 $\mu = 0.1$). Energy distributions of reflected particles (cf. Figs. 4 and 5) at $\vartheta = 60°$ for the *VCC* and *FCC* lattice model show that these distributions depend upon the type of lattice. A distribution curve of nitrogen molecules from iron crystal at $\vartheta = 0°$ is given in Fig. 6. The multilobular kind of distribution curves is determined by the atomic structure

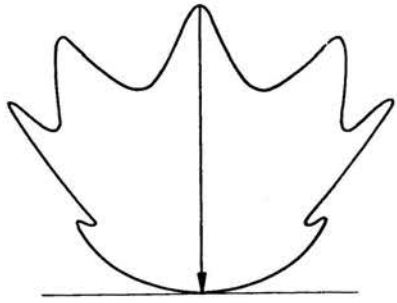

FIG. 6. Angular distribution of reflected molecules (N_2-Fe, incident angle equals 0°).

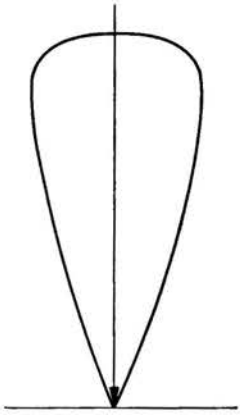

FIG. 7. Angular distribution (N_2-Si).

of the crystal. For the interaction of N_2 molecules with a more dense silicon lattice, we obtain a smooth distribution curve of reflected particles (Fig. 7).

In the particular case of interaction of an argon atom beam with a silver surface, the calculations were realized for interaction parameters approximating to those used in the experimental study [4]. In Fig. 8 is shown a distribution density of reflected particles in qualitative agreement with the experimental curve at $\vartheta = 60°$. The distribution curves for incident energy of $E = 1.4$ev and various angles ϑ are shown in Fig. 9. The lesser

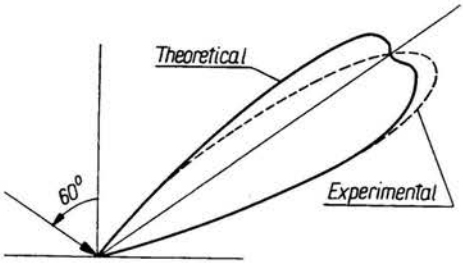

FIG. 8. Angular distribution (Ar–Ag).

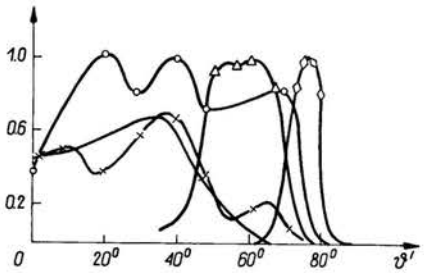

FIG. 9. Angular distribution Ar–Ag, $E = 1.4$ev ($-\vartheta = 0°$, $\times -\vartheta = 30°$, $\circ -\vartheta = 45°$, $\triangle -\vartheta = 60°$, $\Diamond -\vartheta = 75$.

smoothness of the theoretical curves in comparison with the experimental ones — one of which is plotted in Fig. 8 — is connected with the roughness of the surface, the influence of which smoothes out the experimental curve.

A study of the collisions of gas molecules with alloys requires knowledge of the parameters of interaction potentials within the crystal of the alloy. With a certain error, it may be accepted that the combining laws are valid for the internal interaction potential. In this approximation, but with the real structure of the crystal, the calculation of accommodation coefficients was realized for alloys containing two or three components.

In Figs. 10 and 11 are plotted the curves of dependence of energy and momentum accommodation coefficients on the incidence angle ϑ for a copper-aluminium alloy (the

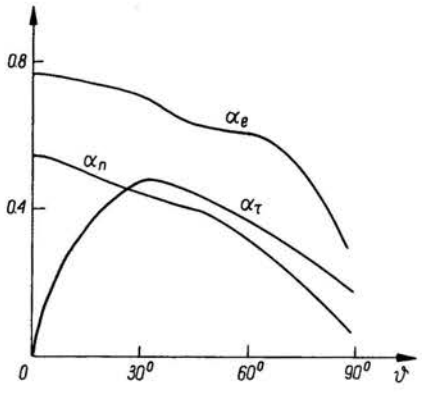

FIG. 10. Accommodation coefficients for two-component alloy.

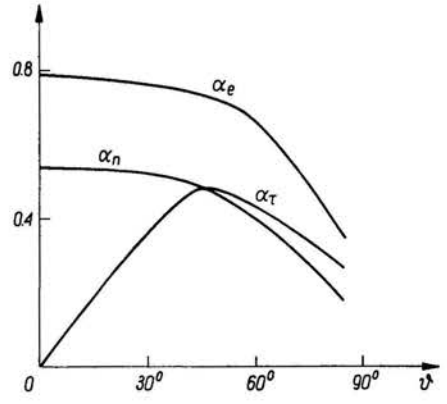

FIG. 11. Accommodation coefficients for three-component alloy.

main component is Al) and steel with considerable content of nickel and chromium. The energy distributions of reflected particles against angle ϑ' measured from the normal to the surface, and azimuthal angle φ', read from one of the crystallographic axes for two values of the initial incidence angle ($\vartheta = 30°$ and $60°$) are drawn in Figs. 12, 13, 14, 15.

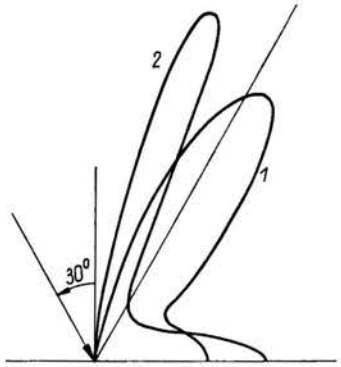

FIG. 12. Angular distributions ($\vartheta = 30°$, *1*-two, *2*-three component alloy).

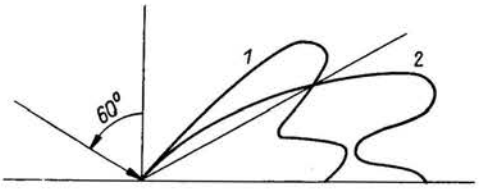

FIG. 13. Angular distributions ($\vartheta = 60°$).

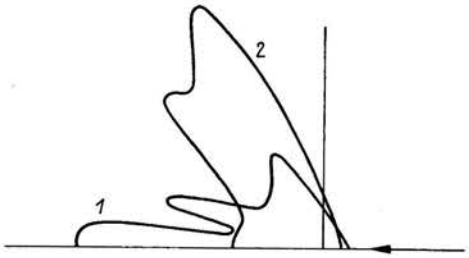

FIG. 14. Azimuthal distributions ($\varphi = 0°$, $\vartheta = 30°$).

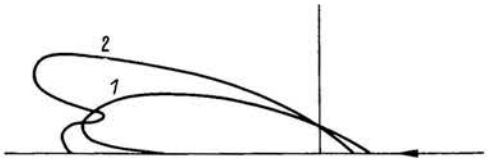

FIG. 15. Azimuthal distributions ($\varphi = 0°$, $\vartheta = 60°$).

In these figures, the curves for the two-component alloy are denoted by 1 and for the three component alloy by 2.

Thus, by making use of a numerical experiment, which is not given in detail here, all parameters of flow of gas molecules reflected from a smooth surface may be obtained. The distribution function of reflected particles may be presented in the form of Tables convenient for numerical solution of the Boltzmann equation. A preliminary study of the molecular beam scattering performed in the numerical experiment gives excellent starting data for designing the measuring apparatus in laboratory or natural experiments. A numerical experiment, after its results have been compared with those of a reliable experiment, may be substituted for the latter when such is very difficult to realize.

It is not possible to take into account the fact that the procedure used in the numerical experiment is standard and a program once prepared can with minimum modifications be used for a whole series of calculations.

The fact that the interaction parameters, obtained by means of numerical modelling, may be used for computation of aerodynamical drag coefficient C_D of the Earth-satellite [5] should be emphasized. For example, using the data concerning the configuration

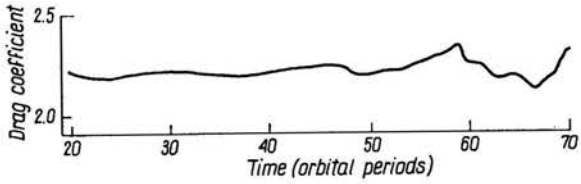

FIG. 16. Aerodynamical drag coefficient for Proton 2.

of the satellite, the surface material and orbital motion for the satellite Proton 2, we obtained the dependence of aerodynamic drag on time, which is shown in Fig. 16 [6].

The comparison of values of C_D obtained by numerical and laboratory [7] experiments shows their qualitative agreement.

References

1. A. A. PYARNPUU, *Computation of monoenergetic gas atom beam interaction with a three-dimensional crystal* [in Russian], PMTF J., No. 2, 162–167, 1970.
2. A. A. PYARNPUU, *Models of rarefied gas interaction with a solid surface* [in Russian] in "Numerical Methods in Rarefied Gas Theory", Comp. Center. Acad. of Sci. of USSR., 119–139, 1969.
3. YU. A. RYZHOV, D. S. STRIZENOV, *On the interaction of atoms with a solid surface* [in Russian], PMTF J., No. 4, 113–117, 1967.
4. W. J. HAYS, *Scattering of argon beams with incident energies up to* 20ev *from a* (111) *silver surface*, School of Engineering and Applied Sciences, Univ. of California, Los Angeles, Rep. No. 7061, July 1970. M. YA. MAROV, A. A. PYARNPUU and G. I. ZMIEVSKAYA, *Gas flow-satellite surface interactions and deduced atmospheric density variations*, Space Research XI — Academie Verlag, 935–939, Berlin 1971.
6. A. A. PYARNPUU and G. I. ZMIEVSKAYA, *Numerical modelling of interaction processes on a satellite surface*, Seventh Int. Symp. on Rarefied Gas Dynamics, Book of abs., **1**, 218–219, 1970.
7. J. W. BORING, R. R. HUMPHRIS, *Drag coefficients for free molecule flow in the velocity range* 7–37km/sec, AIAA Journal, No. 9, 1658–1662, 1970.

COMPUTING CENTER
ACADEMY OF SCIENCES OF U.S.S.R., MOSCOW.

Received April 2, 1972.