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GAS-SURFACE INTERACTION RESEARCH

June 1969

Grumman

RESEARCH DEPARTMENT

GRUMMAN AIRCRAFT ENGINEERING CORPORATION

BETHPAGE NEW YORK

Grumman Research Department Report RE-365

GAS-SURFACE INTERACTION RESEARCH

by

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and

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June 1969

Approved by: *Charles E. Mack, Jr.*
Charles E. Mack, Jr.
Director of Research

FOREWORD

This is the final report on the extension of Contract
NASw-1461 from February 21, 1968 through April 21, 1969. Research
performed under this contract and under the Contractor's inde-
pendent research and development program is summarized herein, and
scientific reports containing full details are referenced. Recom-
mendations for the applications of this type of work, and for
future research in this area are made in an Appendix entitled "On
the Future of Gas-Surface Interaction in Space." This work, like
previous research in this area, has been partially supported by
the NASA Fluid Dynamics Branch, OART. We are grateful to Mr. Al-
fred Gessow, Dr. James Danberg, and Mr. Ira Schwartz for their
help and encouragement over the past six years.

ABSTRACT

Results of research into several problems of gas-surface interaction are summarized. Numerical calculations using a large computer program have been compared with laboratory experiments using a shock tube driven molecular beam apparatus, and remarkable quantitative agreement is evident for Ar/Ag(111) films at about 1 eV. Certain features of both the calculations and the experiments can also be compared with results from other laboratories; these comparisons are also very encouraging. Some differences between theory and experiment for Ne/Ag(111) and in amplitude trends in Ar are indicated, and these differences offer the opportunity to remove some of the shortcomings of the interatomic potential models we are using. Theoretical results on the effects of surface roughness and related efforts providing simple analytical correlations for normal and tangential momentum exchanges are also described briefly. Complete details of these programs are described in separate reports. A description of the current status of theoretical work on associative desorption is given, and the Appendix states the potential uses of and the need for more research on gas-surface interaction.

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INTRODUCTION

Our research over the past seven years has resulted in several different lines of work in gas-surface interaction. Currently active are: 1) experimental work on scattering from laboratory-grade surfaces in a shock tube driven molecular beam facility; 2) calculation of several properties of interactions using a large complex computer theory; 3) correlation of interaction (accommodation) coefficients in simple analytic form for application to engineering problems; 4) investigation of roughness effects; and 5) theoretical investigation of associative reactions at a surface. We discuss each of these efforts in turn, referring the reader to more detailed reports in each instance except the last.

EXPERIMENTAL RESEARCH

We presented a very brief discussion of our recent experimental results in Ref. 1. The results given below are excerpted from a more detailed report on this subject (Ref. 2), which is now in the final stages of preparation.

We have measured the absolute magnitude of the density fields resulting from the scattering of monoenergetic argon beams from freshly deposited, epitaxial silver films. The energies employed are nominally 1 and 2 eV, and we have data near 1 eV for 40°, 50°, and 60° incidence. The data are reproducible to within a few percent when measured with different detectors, and the scattering patterns appear to be stable for times ranging from a few milliseconds to many hours under vacuum ($\sim 5 \times 10^{-7}$ torr). Evidence of sudden degradation occasionally appears (i.e., one run may be radically different from the one immediately before it). We are able to operate in spite of these sudden changes because they are readily detectable and usually do not occur until 6 to 8 runs have been made on a new target. Several possible causes of this behavior will be investigated in the future. We believe the most likely cause to be a small amount of contaminant gas (e.g., H_2O) in the source, the sticking probability of which increases sharply once some of the surface is covered. Another strong

possibility is occasional infiltration of the beam by debris from the shock tube. The time scale for contamination by the background gas in the system has been shown to be much too long to contribute to the observed sudden degradation of signal.

Figure 1 shows the coordinate system used; Figs. 2,3 show our data near 1.0 eV. We estimate the actual beam energy to be 1.1 ± .1 eV, where the scatter represents the variation between runs. The noteworthy features of these measurements are the remarkable agreement, both in and out of plane, with the theoretical calculations performed by Oman (Ref. 3) and the agreement in peak angle direction with the measurements of Romney (Ref. 4) for the same system (see Fig. 5 of this report). The fluxes are very high near the peak, leaving little gas to be scattered far from the peak. The theoretical curves of Fig. 2 were calculated recently, but those of Fig. 3 are from the trajectories calculated for curve a) in Fig. 9 of Ref. 3. In this case we have shown the normalized density, ρ/ρ_i, instead of the normalized flux, $\rho v/\rho_i v_i$, per steradian. We have had more difficulty establishing reproducible density magnitudes at 2 eV, but the peak angle has been measured repeatedly, as shown in Fig. 4. Damage (and/or contamination) seems to occur more readily for this case, and we do not always get the same initial scattering pattern.

We also have some data for Ne/Ag(111) films at several energies from about 0.25 eV to about 1.0 eV. It is much more difficult for us to detect Ne in our system; thus the quality of the data is not yet as good as that of the argon data. The theory (Ref. 3) predicts that Ne scattering should be narrowest at about .25 - .5 eV and much broader than Ar scattering at corresponding energies above this range. Our data indicate that Ne scattering does broaden with increasing energy above about .25 eV, but that it has about the same relative width (and therefore amplitude on a scale of ρ/ρ_i) as the Ar scattering. Unfortunately, these data have not yet been replicated and therefore cannot be relied upon. They nevertheless indicate how similarities and differences between complex computer theory and experiment, applied to several different cases, can point to needed improvements in interatomic potentials and eventually lead to a realistic model for the surface potential field.

The molecular beam used to generate the data discussed above is the product of several years of work, part of which was included in the scope of this contract. Although we have been unable to investigate many interesting beam problems since we wished to give full attention to the scattering experiments, certain important features of the beam had to be investigated thoroughly to ensure integrity of the results. The beam velocity was measured in several

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ways, the most accurate involving time of flight between tandem detectors (density gauges). Radial density profiles of the beam were measured under many different conditions to ensure that the test surface was the only surface that had appreciable beam impingement and that the reflected density measurements did not include any molecules scattered out of the incident beam instead of from the surface. We discovered that skimming at very high incident intensity resulted in extremely large attenuations $[0(10^{-3})]$ across the skimmer, and that the final beam appeared to have a higher velocity (as high as $1.4 v_i$) than that measured ahead of the skimmer and predicted by adiabatic steady-flow expansion laws. We had to understand this effect at least thoroughly enough to distinguish it from the unsteady expansion in the nozzle, which also produces significant increases in velocity at the beginning of a run. It is, apparently, a phenomenon associated with extremely large collision effects, so that the anomalous velocity increment vanishes as intensity is decreased and is not noted under normal (even "lossy") skimmer operation. We discussed the beam calibration problems briefly in Ref. 2, and we hope to cover our work in this area more fully in a future report.

<u>ERRATUM: Numerical Experiments on Scattering of Noble Gases from Single-Crystal Silver</u> [J. Chem. Phys., <u>48</u>, 3919 (1968)]

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The expression for the constant A, given several lines below Eq.(2), was incorrectly transcribed to the manuscript. It should read:

$$A \approx \frac{2}{N} \left[\frac{1}{B} - \frac{1}{3!B^2} + \frac{2}{5!B^3} \cdots \right]^{-1} .$$

The correct form was used in all of the computer programs utilized in applying the method, so no further corrections are necessary in the original paper or in Ref. 1, which employs the same method. I regret any possible inconvenience to users of the method, and I am grateful to Yue Kwong Chiu for calling the error to my attention.

[1] R. A. Oman, in <u>Rarefied Gas Dynamics</u>, Proceedings of the 6th Symposium, edited by L. Trilling and H. Y. Wachman; Vol. II, p. 1331, Academic Press (1969).

COMPUTER CALCULATIONS OF
MONATOMIC GAS-SURFACE INTERACTIONS

A report on our basic computer theory applied to interactions of inert gases with a silver (111) surface was given at the 6th Symposium on Rarefied Gas Dynamics (Ref. 3); it described the bulk of our theoretical work in this contract period. Several new cases (e.g., the theoretical curves of Fig. 2) have since been computed in support of our own laboratory data and for comparison with particular measurements made by Romney (cf. Fig. 4 and Ref. 4). There has been very little need to revise this theory in the past year or so. Its basic limitation as regards the near future is neither in computational technique nor in computer time requirements, but rather in the knowledge of interatomic potentials that it requires. Improvements are always possible, but it has become increasingly obvious to us that the uncertainties in the potentials (in effect, the atomic radius at a particular incident energy level) are large enough to alter the character of the results completely. We believe that experiments will be necessary on several related systems (e.g., He, Ne, Ar, Kr, Xe on Ag) over a broad range of energies. Working with very complex three dimensional calculations, we believe we can find the potential forms that reproduce the experimental behavior.

At this writing, the results of Ref. 3 (and of later cases using the same parameters) seem to explain most of the trends observed experimentally. The predicted transition from thermal scattering to structure scattering at about 1 eV for Ar/Ag(111) appears to be displayed in the direction of the peak angle (cf. Fig. 4) and also in the width of the lobe (cf. Ref. 4). The decrease in peak amplitude with energy that had been predicted above 1 eV does not appear in the experiments so far examined, but since the fluctuations in both laboratory and numerical data seem to affect this measurement most severely, more study is required here. In the case of Ne/Ag(111), the anticipated broad scattering above 0.5 eV has not appeared in our very limited results, although, as predicted, the width does increase with increasing energy in this range. In the light of the long-standing anomaly between observed sharp reflection and predicted broad scattering for room temperature He, we tentatively conclude that the repulsive portion of the potentials does not "soften" as the attractive part becomes weaker. The Lennard-Jones 6-12 potential imposes such behavior somewhat arbitrarily, and it appears to be time to adjust it to produce more realistic energy dependence.

One further comment on the energy dependence in the argon/ silver system is in order. Figure 5 shows that most of the change in peak angle that occurs at high incident energy E_i (Fig. 4) is

due to an increase in tangential momentum exchange, σ_t, although neither the normal nor the tangential momentum has the value predicted by hard cube theory at high energy. The silver (111) face is very tightly packed, so σ_t is quite low at low E_i; but a steady rise with increasing E_i is apparent. We believe this is due to increasing resolution of the atomic configuration (i.e., the atomic radius decreases).

CORRELATIONS FOR MOMENTUM EXCHANGE

It has been demonstrated repeatedly that fairly simple models of the interaction can predict energy exchange quite well. In our previous work we developed a formula based on a simple phenomenological model that correlated our full-scale numerical calculations over a wide range of input conditions (Ref. 5). Goodman (Ref. 6) has also correlated momentum and energy exchanges in hard sphere interactions, using a reduced form of the same formula for the energy.

Recently, we have discovered formulas that predict normal (σ_z) and tangential (σ_t) momentum exchange in simple algebraic form. This has been accomplished by correlating the simplest model (Goodman's hard spheres), using the energy exchange law and Goodman's asymptotic rules (Ref. 6) as starting points, and adding geometric effects deduced by physical reasoning. Appropriate corrections were added to account for soft potentials, lattice thermal motion, and lattice restoring forces. The resulting simple algebraic formulas correlate normal and tangential momenta to a root-mean-square error of 11 and 10.2 percent, respectively, for the 64 cases we have long used as a standard set of results (Ref. 5).

Our correlations of Goodman's hard sphere results are

$$\alpha_e \equiv \frac{E_\ell}{E_i} = \frac{-4\xi\mu \, \cos \, \theta_i}{(1 + \mu)^2}$$

where α's are Goodman's notation, and we use E_ℓ and E_g to denote energy left in the lattice and gas atom, respectively.

$$\sigma_z = 2 - \alpha_n = 1 + \frac{\mu}{1 + \mu} \, \xi^2 P \left[1 - \frac{0.3 \, \mu}{1 + \mu} \frac{\ell}{R} \tan \theta_i \right]$$

$$\sigma_t = \alpha_t = - \frac{\cos \theta_i}{\frac{R}{\ell} + 1} \left[\frac{4\mu}{(1+\mu)(\frac{R}{\ell} + 1)} + 1.2(\frac{R}{\ell}) \cos \theta_i \left(\frac{\mu - 1}{\mu + 1} \right) \right]$$

where $\mu = m_\ell / m_g$, θ_i is the incident angle $(\pi/2 < \theta_i \le \pi)$, R is the atomic radius appropriate to the energy E_i, ℓ is the lattice grid spacing ($\sqrt{2d}$ in our usual notation), P is $\sqrt{1 - \alpha_e}$ (the scalar momentum of the exit gas divided by the incident momentum), and ξ is a geometric parameter defined as

$$\xi \equiv \left[R^2 \sec^2 \theta_i - (\frac{\ell}{2})^2 \right]^{\frac{1}{2}} \Big/ R \sec \theta_i \quad ; \quad \frac{R}{\ell} > \frac{1}{2} \; .$$

The above relationships will be described more fully in Ref. 7, where additional procedures are also given for treating correlations at lower energies. Figure 5 shows the degree to which the low-energy forms of the above formulas fit the calculated results for Ar/Ag(111) at 50° $(\theta_i = 130°)$ incidence. Figures 6 and 7 show the scatter in the correlation of 64 test cases from Ref. 5.

We think that these simple formulas will be useful in at least three ways. First, they enable us to see in analytic form the ways in which each variable affects the results. Often we can see how such dependencies are associated with a physical process. Second, there is now a quite simple way to get an

answer to engineering problems if one can guess the input variables well enough (e.g., the atomic radii, the surface Debye temperatures, etc.). Third, we now have a platform from which to attack new problems such as parametric modeling (cf. Hurlbut and Sherman, Ref. 8) and surface roughness effects (see the following section).

SURFACE ROUGHNESS

Since no real surface is perfectly smooth, surface irregularities have long been invoked as a rationalization for the use of diffuse wall reflection models in rarefied gas problems. Some studies of roughness effects have been made previously, but we have always considered it essential to incorporate in the study of roughness a realistic model of the local interaction on a flat facet. The momentum exchange model described above supplies the analytic dependence of the momenta on the local incidence angles. This makes possible a statistical weighting process to treat different surface models.

One can describe a surface by its "angle distribution function" and its "height distribution function." These are, respectively, the relative probability of encountering the surface element at a particular inclination or height relative to the reference plane of the surface. If we know the interaction laws for a locally flat element at arbitrary inclination, we can fold the functional dependence of the interaction with the distribution of inclination to determine mean interaction effects for first collisions. Shadowing, the preferential weighting of higher surface elements relative to those in valleys, can be done rigorously only if the height distribution is specified; but it can be modeled by relatively simple

functions. The modeling of second and higher-order collisions becomes very difficult if one attempts to go beyond a very simple model (e.g., all molecules emitted "downward" are randomized or, alternatively, focused in a particular direction, as in the work of Jackson, Ref. 9).

Several different ways of specifying surface angle distributions have been employed in our first look at roughness effects. These are

1) An Isotropic Surface. The probability of encountering the surface at θ_s is constant for all θ_s between 0 and $\pi/2$.

2) A Gaussian Surface:

$$f(\theta_s) = A \exp\left\{- \frac{(\theta_s - \theta_o)^2}{\bar{\theta}^2}\right\}$$

where θ_o and $\bar{\theta}$ are disposable parameters, and A is the appropriate normalizing constant.

3) A Saw-Tooth Surface:

$$f = \delta(|\theta_s - \theta_o|)$$

($\theta_o = 0$ gives a flat surface).

4) Each of the above with simple shadowing functions.

We have employed the correlations of Goodman's data that are given in the previous section for the "flat surface" laws, and have

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computed several cases. One set of these results is shown in Fig. 8.[*] It is important to realize that the computed roughness distributions are three dimensional in that they are integrated over a uniform distribution of azimuth angles. As yet no roughness calculations have been done with momentum rules for lower energies.

The results shown in Fig. 8 are fairly typical of the others we have examined. The smooth surface results show that the calculations recover reasonably accurately Goodman's results for force coefficients. The tangential momentum is, of course, affected by roughness more strongly than is the normal momentum, which seems remarkably insensitive to radical differences in roughness.

A complete development of the theory of the roughness investigation and additional results for different cases will be given in Ref. 10.

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[*]The abscissas in Figs. 8a and b show θ_i as the supplement of the θ_i definition employed previously. $\theta_i = 0$ is impact from the surface normal direction.

ATOMIC RECOMBINATION AT A SURFACE AND
ITS EFFECT ON SATELLITE AERODYNAMICS

It has been demonstrated repeatedly that adsorbed contaminants can have a very significant effect on gas-surface interaction. We find that the largest unknown in the prediction of aerodynamic drags and torques, particularly under orbital conditions, is the surface condition. Roughness, the other major factor in the condition of real surfaces, can be treated statistically, but the state of contamination poses some very special problems.

If the surface is clean, we can expect an interaction under orbital conditions that will give moderately broad, generally specularly directed, scattering in which the capture (i.e., adsorption) of incident particles is limited to atoms of oxygen with about a 0.30 sticking probability. The energy exchange of the remaining components would be reasonably approximated by the familiar hard sphere law, with perhaps some small corrections to account for non-normal incidence and lattice restoring forces. A consequence of this line of reasoning is that to reduce drag, heavy atomic weights in the surface (and high Debye temperature in some cases) would be helpful for surfaces at low inclination to the free stream or facing aft. For surfaces facing forward, lowest drag results from having light atoms at the surface.

But for most cases we do not expect the surface to be clean. It may be launched dirty, in which case time and the space environment can be expected to produce a continuous change in gas-surface

interaction as the surface loses species in the order of increasing

binding energy. A problem of special interest is the steady state

case of space exposure, in which the crucial question appears to be

the relative rates of adsorption and desorption of atomic oxygen.

It is very probable that after some time O atoms would replace

all of the other adsorbed contaminants.

Of all the species present in high concentration in the

50 - 1000 km region (where aerodynamic effects are most impor-

tant), the one with the highest probability of sticking to a sur-

face is O. Since one O atom will combine with another with a

high binding energy (5 eV) and form a roughly equivalent bond

with many possible surface atoms, the possibility of an important

desorption mechanism lies in the O - O recombination. The energy

released by the formation of O_2 may or may not become available

to desorb the product molecule, which would have a much lower

(e.g., ~ 0.1 eV) binding energy with most surfaces. If such a

process is not likely, the surface will become covered with O in

a very short time. A crude analysis of the kinetics of surface

encounters indicates that if the reaction cross section (for as-

sociative desorption) is of the order of the size of an adsorption

site, the equilibrium coverage will be a strong function of the

angle of incidence. For grazing incidence, the equilibrium O atom

coverage might be a small fraction of a monolayer. With a fraction

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Θ of a monolayer covered, a reaction cross section Σ, N adsorption sites per unit area, a sticking probability of η_s on a bare site and zero on an occupied one, and an incidence angle θ (measured from the normal), we can write, for equilibrium:

$$\eta_s[1 - \Theta] - \frac{8}{\pi} \Theta N \Sigma \tan \theta \approx 0$$

The second term in the above equation includes an estimate of the probability of passing near enough to an adsorbed atom to react and desorb both atoms as one molecule. Solving for Θ, we get

$$\Theta \approx \frac{1}{1 + \frac{8}{\pi} \frac{N}{\eta_s} \tan \theta} \quad,$$

showing that arbitrarily low coverages are possible by this mechanism alone.

Because we believe this associative desorption might become one of the most important questions in gas-surface interaction, and since it is related to possible future extensions into the area of surface catalysis, we have begun to study this process with our computer models. The principal difficulty is the primitive state of our knowledge of interatomic potentials. If we can construct a consistent model for the potential surfaces of three mutually interfering atoms, the computation of representative

interactions at the satellite energy level will not present any new problems. For the results not to be misleading, however, we must be able to treat several rather different potential models and display the expected reaction mechanics for each. Confidence in the final outcome will depend greatly on how sensitive the results are to details of the potential surfaces. This is quite different from the problems we have treated thus far, in which only the gross features of the potentials have had important effects on the results.

The method of analysis is based on a modification of our basic gas-surface program for diatomic interactions (described in the proceedings of the Fifth Symposium on Rarefied Gas Dynamics, 1966). The initial conditions in the program are modified so that one atom is initially incident on the surface while the other is initially adsorbed near the impact site. In addition, a three-body potential has been constructed in a general form that satisfies all of the necessary limit constraints. For example, one gas atom is influenced by the other atom through a strong chemical bond that is continuously diminished as either gas atom approaches the lattice. The bond of either atom to the bulk is similarly diminished as the distance between gas atoms decreases. In the limit of interatomic distances corresponding to the molecular ground state, the gas-surface bond for each atom is half that of a molecule. We

can then vary the shape of the transition curves between the above limits to test the effects of changes in the details of the interatomic potentials on the cross section for the associative reaction.

We have performed the necessary changes in the main program, and have employed to date only the following form for the interatomic potential:

$$\Phi_A = \tfrac{1}{2}\,\phi_{mL}(r) + \omega_j(r_j)\phi_{AA}(r_i) + \omega_i(r_i)\phi_{AL}(r_j) \quad , \qquad (1)$$

where

Φ_A	is the total potential of a gas atom
ϕ_n	is a contribution from the nth type of interaction
r_j	is the distance between the atom and the lattice
r_i	is the distance between gas atoms
r	is the distance between the mass center of the two atoms and the lattice
$\omega_n(r_n)$	is a weighting function used to attenuate the interaction that competes with the nth bond

and the subscripts are

A	atom
m	molecule
L	lattice.

Equation (1) is not a completely general form for the potential, but it allows for a considerable range of behavior by

assuming different forms for the weighting functions. Boundary

conditions on the ω's are:

$$\omega_j(\infty) = \omega_i(\infty) = 1$$

$$\omega_i(R_m) = 0 \qquad \text{(at molecular separation)}$$

$$\omega_j(R_{AL}) = 0 \qquad \text{(when one atom is adsorbed)} \quad .$$

We have employed for our first trial cases the functions:

$$\omega_i(r_i) = 1 - b\, e^{-c(R_m - r_i)^2}$$

$$\omega_j(r_j) = 1 - B\, e^{-C(R_{AL} - r_j)^2}$$

where the new constants b, B, c, and C are parameters.

We have run a few test trajectories with the program described
above. Results showed a few minor flaws that need attention, but
they were generally quite satisfactory. We have been forced to sus-
pend activity in this area because of the demands of other work on
this project. We believe that the issues involved are sufficiently
important to justify continued effort along these lines, in spite
of the fact that the approach may ultimately prove to be fruitless.
The necessary condition that results be proved to be insensitive
to the shapes of the weighting functions offers the hope but not
the promise of ultimate validity.

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SURFACE-ORIENTED
COORDINATES

APPARATUS-ORIENTED
COORDINATES

DETECTOR
PLANE

PLANE OF
INCIDENCE

TARGET AT ORIGIN WITH SURFACE NORMAL
ON Z-AXIS IN BOTH SYSTEMS
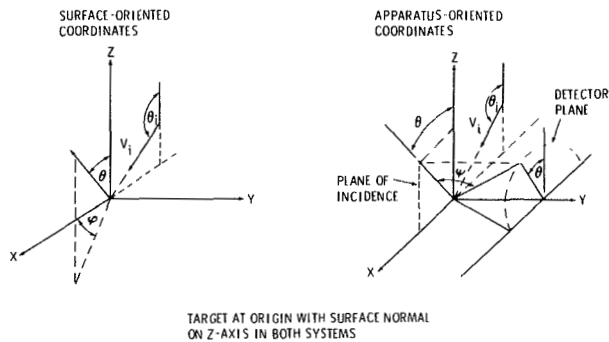
Fig. 1   Coordinates for Comparison of Theoretical
and Experimental Scattering Patterns

Ar/Ag (111) E_i   1.0 eV

40° INCIDENCE
FILLED SYMBOLS, ψ   30°
OPEN SYMBOLS, ψ   0°

IN-PLANE PROJECTED DETECTOR ANGLE, θ
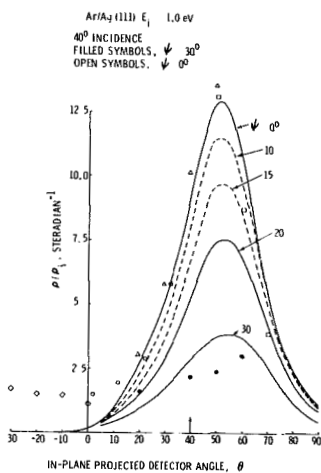
Fig. 2   Comparison of Theoretical and Experimental
Density Fields for 1 eV Argon on (111)
Silver at 40° Incidence

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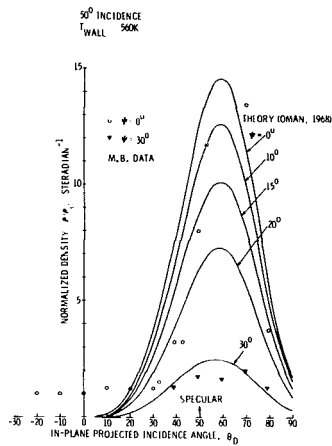
Fig. 3   Comparison of Theoretical and Experimental
         Density Fields for 1 eV Argon on (111)
         Silver at 50° Incidence
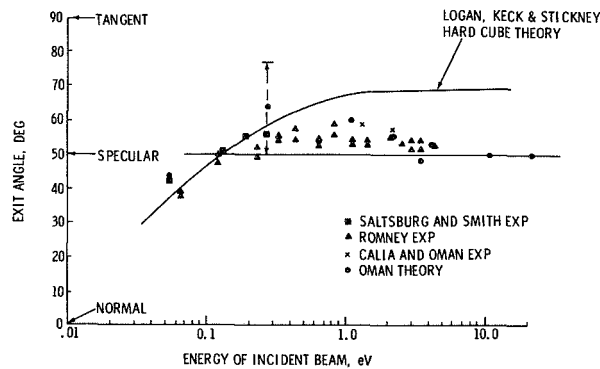
SCATTERED PEAK DIRECTION AT 50° INCIDENCE
ARGON/(111) SILVER

Fig. 4   Comparison of Peak Directions from
         Several Laboratories

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SYMBOLS ARE FROM CALCULATIONS
CURVES ARE CORRELATION EQUATIONS

VALUES FOR SPECULAR
REFLECTION WITH E_g/E_i = .7

$\sigma_z = 1 + \left|\frac{V_z}{V_{zi}}\right|$

E_g/E_i

$\sigma_t = 1 - \left|\frac{V_x}{V_{xi}}\right|$

INCIDENT ENERGY, (eV)
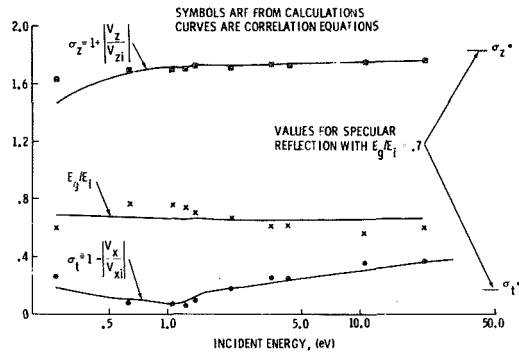
Fig. 5   Energy and Momentum Coefficients for
Argon/(111) Silver at 50°   Incidence

PREDICTED NORMAL MOMENTUM CHANGE, σ_{zP}

ACTUAL NORMAL MOMENTUM CHANGE, σ_z
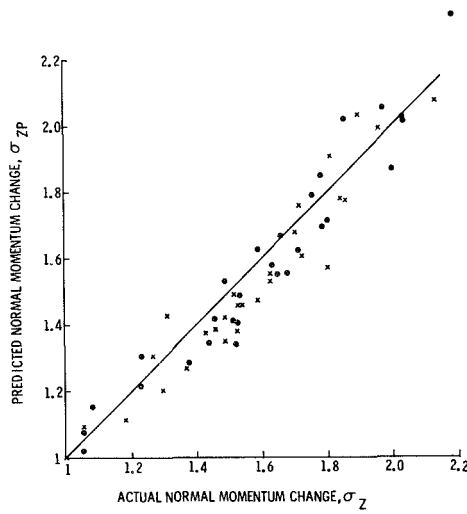
Fig. 6   Phenomenological Model Correlations of
Normal Momentum for a Variety of
Interactions
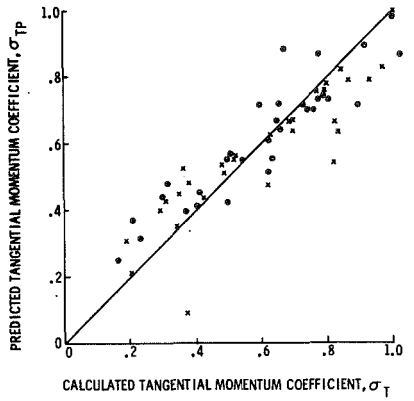
Fig. 7   Phenomenological Model Correlations of
         Tangential Momentum for a Variety of
         Interactions
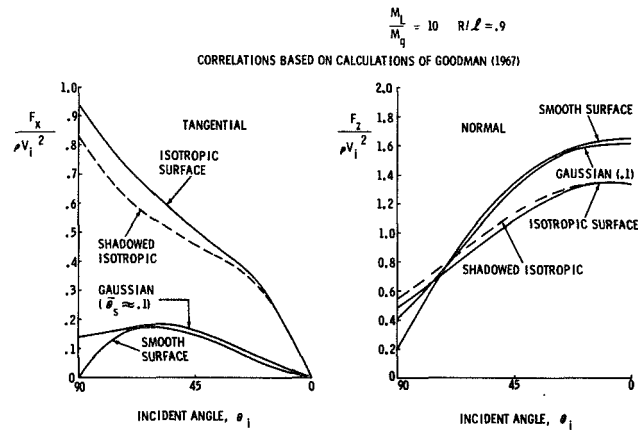
Fig. 8   Effects of Surface Roughness on Forces
         for Hard Sphere Interactions

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APPENDIX

ON THE FUTURE OF GAS-SURFACE
INTERACTION IN SPACE FLIGHT

by

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In making a plea that applied research on gas-surface inter-
action be given a higher priority I assume two obligations: first,
to show an underrated requirement, and second, to show promising
lines of development. I would welcome an opportunity to give de-
tails and documentation for the brief that follows.

I.   The Need

There is a lot more to the need for gas-surface interaction
research than the determination of drag coefficients on blunt
satellites. From where I sit, aerodynamic torques on large sat-
ellites are the primary concern. Also very important are impinge-
ment forces on structure (particularly solar paddles) from control
rockets, and the contamination of sensitive surfaces (windows,
solar cells, thermal coatings, etc.) by effluents and by rocket
plumes.

It appears to me inevitable that the nation will continue to conduct manned orbital experiments, that the vehicles will get larger, and that the missions will get longer. For larger satellites, aerodynamic forces become **increasingly** important through torques, and decreasingly important through orbital decay (drag). Large solar paddles (as large as 5,000 ft^2) and/or radiators appear to dominate space station designs now being considered. The aerodynamic torques on such designs are very large, often exceeding those of gravity gradients for 200 n mi altitudes, even if the additional unbalance of forces due to shadowing is not considered. Shadowing, which tends to be important at glancing incidence, can increase peak torques another order of magnitude. Because satellite missions usually require controlled orientation, active stabilization must be employed. The reaction control system fuel expenditures for one such design integrate to 10^4 lbs/yr, employing inertia wheels to store the alternating components of angular momentum. The diurnal "bulge" of the atmosphere is the primary cause of the high level of bias torque in a complete orbit. The momentum exchanges at surfaces (and therefore the aerotorques) can differ by large amounts (variations of an order of magnitude are quite possible) for different types of gas-surface interactions when the local incidence is near grazing, even for engineering (i.e., rough) surfaces. The stakes in many mission analyses are

high enough to consider varying the geometry or surface material of the paddles to aid in attitude stabilization as confrontation angles change. To do this, we must have reliable prior knowledge of the gas-surface interaction at appropriate energies.

In addition to atmospheric interactions on space stations, we must recognize other problems. Impingement of propulsion plumes on vehicle surfaces can cause major problems (OAO-2 has measured roll-jet torque degradation that varies between 26 and 42 percent, which can be explained by plume impingement and a greater-than-specular normal force on the adjacent solar paddle). One might wish to design deliberate plume impingement to achieve significant torque multiplication. Long-term effects of contaminants deposited on windows and solar paddles can be serious, and their prediction requires knowledge of sticking probabilities. We have not yet really begun to look at using lift and drag modulation in rarefied atmospheres for orbital plane changes, booster recovery, and/or low-altitude satellite operations. If such activities are feasible, they will demand a great deal better GSI technology than we now possess.

II. A Plan of Action

Although an array of effective theoretical methods is now available, there are two key barriers to reliable predictions for

space flight conditions. First, the interatomic potentials between gas and solid atoms are not known well enough in the strongly repulsive regions that are important above 1 eV; and second, we do not know what long-term exposure to atomic oxygen will do to the state of contamination of typical surfaces. There are, of course, many other questions, but these two are in my opinion the sources of the greatest uncertainty in aerodynamic problems. Numerical methods of great complexity and simpler physically-based theories that explain the results of the numerical computations in various local regions seem adequate to most needs. Surface roughness effects can be modeled with statistical methods, and contaminants can be modeled if we know them. But no theory can overcome lack of knowledge of the surface situation.

We know that the interatomic potentials will look very much like hard spheres at high energy, but we do not know the sizes of the spheres for given species at a particular energy! The exciting recent agreement of experiments from our own laboratory and from Princeton (Romney) with our theoretically predicted density fields for argon on epitaxial silver films has indicated that our guesses for the Ar/Ag potential are pretty close; but Ne/Ag experiments indicate that some features of that potential are not as we predicted. Some of the trends predicted for Ne/Ag are observed, but the scattering is narrower than predicted. It

appears that results, at least in the eV energy range, are quite

sensitive to small changes in the size of the atoms. With careful

calculations for different potentials and careful experiments, we

can discover the important features of the real potentials.

We must also learn what long-term exposure to atomic oxygen

incident at several eV in hard vacuum (i.e., in the space en-

vironment) does to the surface condition. After a suitable ex-

posure in space, is a full monolayer of tightly bound O formed

on the surface, or does the energetically favored association of

two O atoms form a weakly bound molecule and "scrub" the surface?

If the surface is scrubbed, its reflection laws will be very dif-

ferent from one covered with atomic oxygen, which has lower surface

mass and a much stiffer bond (high Debye temperature) than a typical

metal. There is some hope that informative calculations can be done

on this question, but the final answer must await results from space

experiments.

More and more we find that glassy surfaces are used on vehicles:

solar cells, windows, and surfaces for long-term thermal control

(Optical Surface Reflector). No one knows a way to characterize

the surface structure of glass, nor is there even a way to determine

the surface composition of a given glass. By directing our experi-

ments to glassy surfaces, we can learn how solar cell surfaces will

"look" to incident atmospheric species.

III. Using the Results in Gas Calculations

It is particularly frustrating to note that only a minor
fraction of reports on rarefied gas-dynamics make an attempt to
employ modern knowledge of the wall boundary condition. Para-
metric modeling (e.g., Schamberg, Nocilla, Epstein) supplies a
vehicle through which this can be done, by reflecting the re-
sults of detailed GSI investigations in the intelligent deter-
mination of parameters. There are excellent indications that
matching the major moments (energy, two in-plane momenta, and
a momentum spread) can provide sufficient restriction to repre-
sent parametrically the distribution function of wall molecules
in a form compatible with a typical gas-dynamics analysis and
that at the same time reflects the realities of gas-surface be-
havior.

In summary, I feel we must not ignore the need for knowledge
of gas-surface interactions in future space operations, and we
must ensure that provision is made today to provide some of the
pivotal answers. The funding required is relatively small, but
continuity of effort is essential.

Research Department Report RE-365 Unclassified

GAS-SURFACE INTERACTION RESEARCH by R. A. Oman and V. S. Calia, Fluid Mechanics Section, June 1969.

Results of research into several problems of gas-surface interaction are summarized. Numerical calculations using a large computer program have been compared with laboratory experiments using a shock tube driven molecular beam apparatus, and remarkable quantitative agreement is evident for Ar/Ag(111) films at about 1 eV. Certain features of both the calculations and the experiments can also be compared with results from other laboratories; these comparisons are also very encouraging. Some differences between theory and experiment for Ne/Ag(111) and in amplitude trends in Ar are indicated, and these differences offer the opportunity to remove some of the shortcomings of the interatomic potential models we are using. Theoretical results on the effects of surface roughness and related efforts providing simple analytical correlations for normal and tangential momentum exchanges are also described briefly. Complete details of these programs are described in separate reports. A description of the current status of theoretical work on associative desorption is given, and the Appendix states the potential uses of and the need for more research on gas-surface interaction.

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