VII. PHYSICAL ELECTRONICS AND SURFACE PHYSICS*

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A. SIMPLE CLASSICAL MODEL FOR THE SCATTERING OF GAS ATOMS FROM SOLID SURFACES

1. Introduction

For the case of gases of extremely low density (i. e., for free molecule flow), the transfer of momentum and energy between the gas and a solid surface depends entirely upon the nature of the collisions of individual gas atoms with surface atoms. A satisfactory theory of this interaction has not yet been established. The principal objective of the present study is to formulate a simple model whose behavior agrees qualitatively with the experimental data for the scattering of a beam of gas particles from a solid surface.

The following symbols are used:

u = velocity of gas particle

u_n = component of velocity of gas particle in direction normal to surface plane

u_t = component of velocity of gas particle in direction tangential to surface plane

v = velocity of surface atom (assumed to be in direction normal to surface plane)

M = mass of gas particle

m = mass of surface atom

μ = mass ratio, M/m

T_g = temperature of gas beam

T_s = temperature of surface

θ_o = incident angle (measured from surface normal)

θ_1 = outgoing angle (measured from surface normal)

η = angular deviation of the maximum of the angular distribution of the scattered particles from the specular direction.

(All angles are measured in the plane containing both the incident beam and the surface normal.)

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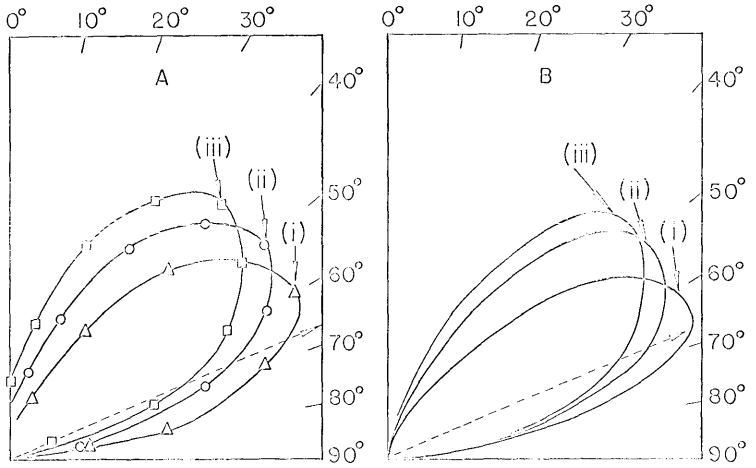

Fig. VII-1.

Temperature dependence of scattering patterns.
(A) Experimental results for Ar on Pt.[1]
(B) Analytical results.
In both cases, $\theta_o = 67.5°$ and $\mu = 0.2$
Curve (i): $T_s/T_g = 1.24$;
Curve (ii): $T_s/T_g = 2.57$;
Curve (iii): $T_s/T_g = 3.68$.

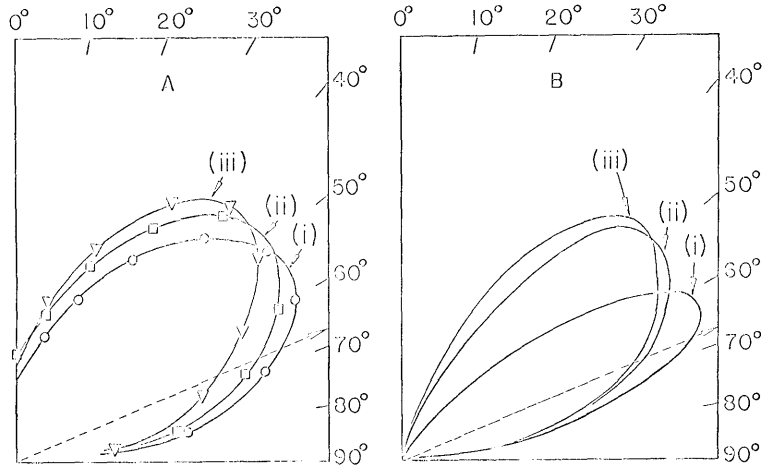

Fig. VII-2.

Mass dependence of scattering patterns.
(A) Experimental results for He, Ne, and Ar on Pt.[1]
(B) Analytical results.
In both cases, $\theta_o = 67.5°$ and $T_s/T_g = 3.60$
Curve (i): $\mu = 0.02$ (He on Pt)
Curve (ii): $\mu = 0.1$ (Ne on Pt)
Curve (iii): $\mu = 0.2$ (Ar on Pt).

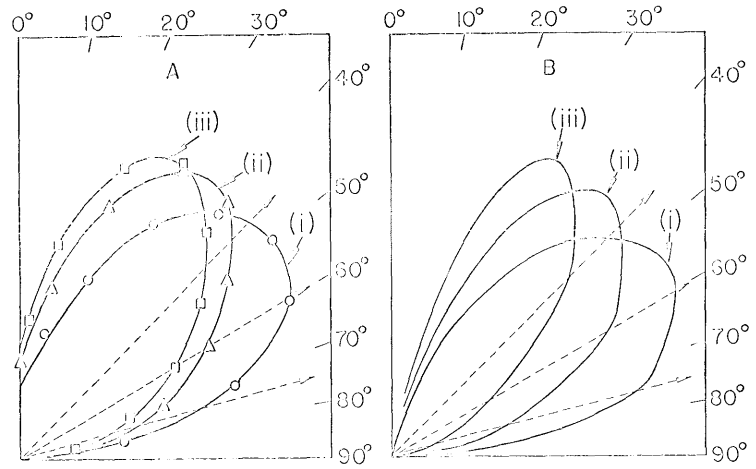

Fig. VII-3.

Incident angle dependence of scattering patterns.
(A) Experimental results for Ar on Pt.[1]
(B) Analytical results.
In both cases, $\mu = 0.2$ and $T_s/T_g = 3.67$
Curve (i): $\theta_o = 75°$;
Curve (ii): $\theta_o = 60°$;
Curve (iii): $\theta_o = 45°$.

The experimental results which are relevant to the present study are the lobular scattering patterns, examples[1] of which are shown in Figs. VII-1A, VII-2A, and VII-3A. Most of the available experimental results, for a variety of different gases on a variety of different surfaces, may be described by the following characteristics:

1. $\frac{\partial \eta}{\partial T_s}$ is positive
2. $\frac{\partial \eta}{\partial T_g}$ is negative
3. $\frac{\partial \eta}{\partial M}$ is positive
4. $\frac{\partial \eta}{\partial \theta_o}$ may be positive or negative

Characteristics 1, 3, and 4 are illustrated in Figs. VII-1A, VII-2A, and VII-3A, respectively. One further characteristic which seems to hold is $\eta \to 0$ as $\theta_o \to 0$.

2. The Model

The simple classical model which is used is based upon the following principal assumptions: (i) the interaction of a gas atom with a surface atom may be represented

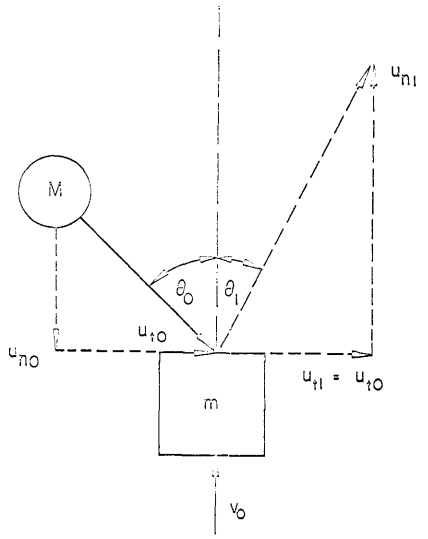

Fig. VII-4. The "Hard-Cube" model.

by an impulsive force of repulsion; (ii) the gas-surface intermolecular potential is uniform in the plane of the surface (hence the interaction does not change the tangential velocity of the gas particle); (iii) the surface atoms are represented by independent particles confined by square-well potentials; (iv) the surface atoms have a Maxwellian velocity distribution. The model incorporates many of the same features as that proposed

by Goodman.[2] As a result of these assumptions, the model is simplified to the extent that it contains no adjustable constants. In order to combine assumptions 1 and 2, it is convenient to think of the surface atoms as cubes oriented with one face parallel to the surface plane and with motion only in the direction normal to the surface plane. Each gas particle interacts with just one of these cubes (Fig. VII-4).

3. Summary of the Analysis

Since the details of the analysis require considerable space, we have chosen to omit them here. A more complete report has been submitted for publication in the Journal of Chemical Physics.

The analysis has been carried out in two stages. In the first stage, the analysis is simplified by representing the velocities of the gas and surface particles by mean values instead of considering the velocity distributions of each. In the second stage, the velocity distributions are considered.

The first stage analysis yields only the approximate angular position of the maximum of the scattering pattern, and hence η, as given by the following expression:

$$\eta = \theta_o - \cot^{-1}\left\{\cot\theta_o\left[\left(\frac{1-\mu}{1+\mu}\right) + \frac{16}{9\pi}\left(\frac{\mu}{1+\mu}\right)\frac{T_s}{T_g}\frac{1}{\cos^2\theta_o}\right]\right\} \qquad (1)$$

An indication of the behavior of Eq. 1 is given in Figs. VII-5 and VII-6.

The full analysis involves integration over the distribution functions of the gas and surface atoms, and this has been done partly by numerical computation. Some of the

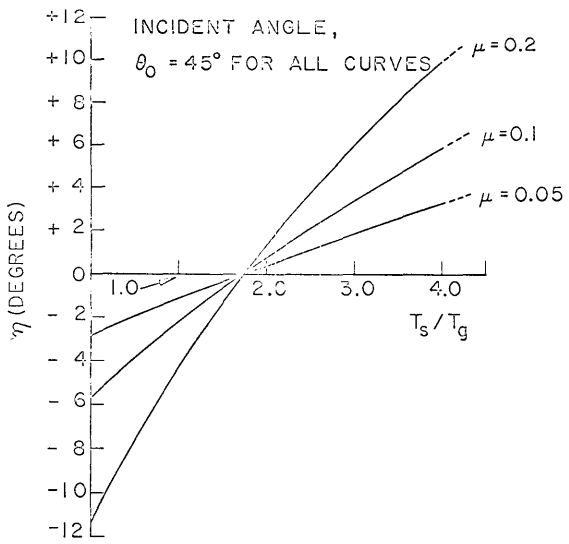

Fig. VII-5. Characteristics of the approximate analysis: The temperature dependence of η, the angular deviation from the specular direction, for several values of the mass ratio μ.

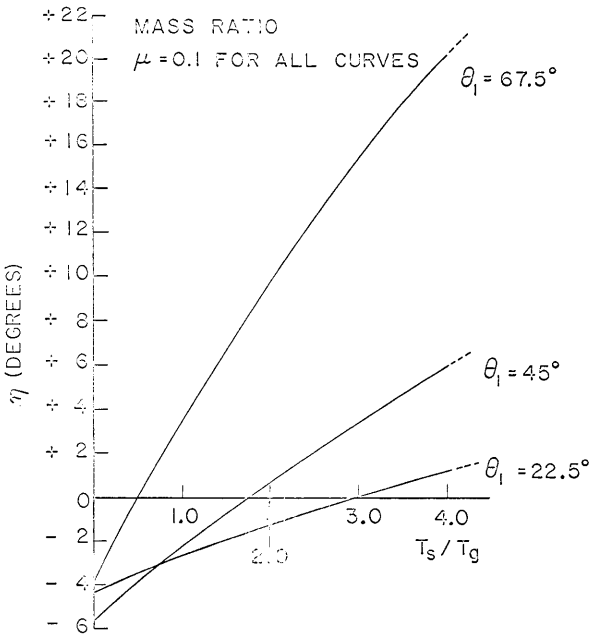

Fig. VII-6. Characteristics of the approximate analysis: The temperature dependence of η, the angular deviation from the specular direction, for several values of the angle of incidence, θ_o.

results are shown in Figs. VII-1B, VII-2B, and VII-3B so that they may be compared with the corresponding experimental results.

4. Conclusions

It is found that the results for η given by Eq. 1 are in resonable agreement with the results from the full analysis. The results from the full analysis are in good qualitative agreement with the experimental results as illustrated in Figs. VII-1, VII-2, and VII-3. Significant quantitative results are not expected from such a simplified model. The good qualitative agreement does indicate, however, that this model may contain the principal mechanisms of the interaction. The results may also be considered as some indication that the general nature of the experimentally observed scattering patterns is not dominated by the precise form of the intermolecular potential or by the topographical form of the atomic surface.

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References

1. J. J. Hinchen and W. M. Foley, "Scattering of Molecular Beams by Metallic Surfaces," in Rarefied Gas Dynamics, Proceedings of the Fourth International Symposium, edited by J. H. deLeeuw (Academic Press, Inc., New York, 1965).

2. F. O. Goodman, J. Phys. Chem. Solids 26, 85-105 (1965).