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MATERIALS FOR FRICTION DRAG REDUCTION THIN FILMS

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SUMMARY

This paper considers that friction drag reductions, in aerospace vehicles, could result from the use of external surfaces thin film coverings with atomic level smoothness. The dynamics of the gas-solid surface interactions, the adsorption phenomena, and the effects of the surface atomic structure on adsorption forces are discussed in order to identify the most adequate materials for such an application. It is concluded that some heavy transition metal halides and dichalcogenides, with "Van der Waals" layered crystalline structures, represent an adequate starting point for further research.

1. INTRODUCTION

The scattering of molecular beams produced by single crystal surfaces in vacuum, show in most cases, velocity distributions having zero mean values of the scattered velocity tangential component. However, in some cases, such as He scattering by LiF or Pd 111 surfaces [1], most gas molecules are elastically scattered resulting in a non zero mean value.

Also in the last decades, the micro electronic device technology brought with it new thin film manufacturing processes [2], which permit to extrapolate for the near future the possibility of obtaining large surfaces with atomic level smoothness.

These considerations suggest, new possibilities of friction drag reductions in aerospace vehicles [3], that will be conditioned to:

- a) The determination of the thin film material properties, required to obtain the elastic scattering of air molecules.
- b) The development of manufacturing and application methods, of large atomically smooth thin film surfaces made with these materials.

Considering the benefits to be obtained in terms of airplane fuel economies, and low orbit satellite life-times, the present work try to investigate the first condition (a), so that with further research on (b), the predicted drag reductions can be experimentally verified.

2. FRICTION DRAG

In aerodynamics, the component in the flow direction of the resultant of all tangential to body surface forces, that is of friction forces, is denominated friction drag.

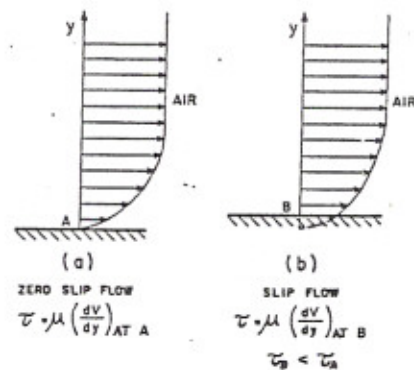
For elongated and "streamlined" bodies such as airplanes, the friction drag can be responsible, at cruising speed conditions, for the major part (around 60%) of the total drag and so of the fuel consumption.

Even for rather blunt bodies, like satellites, when in a low orbit, (below 700 Km), and equipped with large surface solar panels, the friction drag may be significative, 10 to 20% of the drag, and so contribute to their orbit decay.

In continuum fluid mechanics, that is Knudsen Numbers $KN \ll 1$, the friction forces can be computed for various flows regimes, using the "Boundary Layer Theory" [4], which assumes that the relative fluid velocity goes to zero at the surface (zero slip condition, see Fig. 1) and the known "Newton" equation:

$$\tau = \mu \cdot dV/dy$$

where τ is the tangential shear stress, dV/dy the velocity gradient at the surface normal direction and μ is the fluid viscosity.



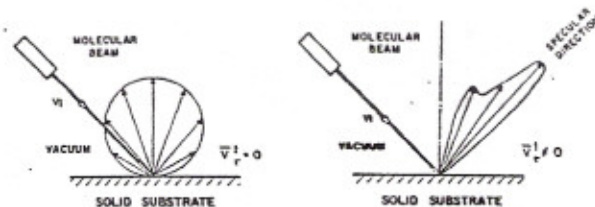
a) zero slip flow b) flow with slip

Fig. 1 - Boundary Layer Profiles.

For rarefied fluid dynamics ($KN > 1$), the friction forces are computed as function of the estimated tangential momentum accommodation coefficient values, which in satellite aerodynamics practical drag estimations [5] are usually assumed as unity, that is: a complete accommodation.

It must be emphasized that in both cases, either for the boundary layer zero slip or for the unit accommodation coefficient, a diffuse reflection of the fluid by the surface, with zero mean value for the tangential reflected velocities of the fluid molecules, is implicitly assumed.

Any possible deviation of this condition towards a more elastic lobular or "specular" reflection (see Fig. 2) will modify these assumptions and result in lower friction force values.



a) diffuse reflection b) Lobular reflection

Fig. 2 - Molecular Beam Scattering

3. DYNAMIC INTERACTIONS

3.1 Mass Effects:

Although the dynamic interactions between atoms and molecules and solid surfaces have been extensively studied [6] this is a rather complex subject, which explains the different theoretical models and some conflicting experimental results found.

The classical mechanics models, such as "hard cubes", "soft cubes", etc, suppose a zero tangential momentum transfer and a simple and accurate model giving the theoretical computation of the tangential momentum accommodation, seem not to be available.

Elaborate numerical simulations [7] and dissipative quantum phenomena [8], such as

electron hole pair, etc., are to be considered to obtain quantitative results.

A simple, but crude approach is the use of the classic "Baule" rigid spheres model [1], which allow the evaluation of the energy accommodation coefficient as function of gas temperature and of the gas and solid atomic masses.

Due to any tangential to normal, and translational to rotational, momentum transfers during gas molecules surface collisions, a low energy accommodation do not implies in a low tangential accommodation, but nevertheless, it is a necessary condition for it.

The "Baule" model shows that in order to increase the elastic reflections, the solid surface atoms must be much more heavier than the gas atoms, and molecules, and it explains elastic scattering results obtained in vacuum, for the helium on different single crystal surfaces.

The effects of the atomic layers below the surface is more evolved and is related to the "phonon" characteristics of the solid substratum.

An extension of the previous mechanical reasoning, indicates that heavier inner atoms, in special if strongly bonded to surface atoms, will contribute to the reduction of "phonon" excitations and to reduce the energy accommodation.

The conclusion is that for aerodynamic drag reduction purposes, only materials with heavy surface atoms and high specific densities shall be investigated.

3.2 Contamination Effects

Another very important aspect, which comes from the study of the dynamic interactions is the effect of the presence of adsorbed species on the surface.

In scattering experiments with elastic reflections, the contamination of the surface, including by the adsorption of low energy gas atoms and molecules, lead to the reduction in the intensity of these elastic reflections.

In all practical applications at normal atmospheric conditions the surface contamination by the air constituents, including water molecules and by solid dust particle of all sizes and shapes, is unavoidable.

A partial solution to this problem, seems to be the reduction of the surface adsorption forces. The reasoning is that

the reduction of adsorption forces and of their tangential component, will reduce the contamination level, and also result in loosely adsorbed species that could easily "slip" along the surface, with less momentum exchange.

4. ADSORPTION FORCES

4.1 Surface Energy

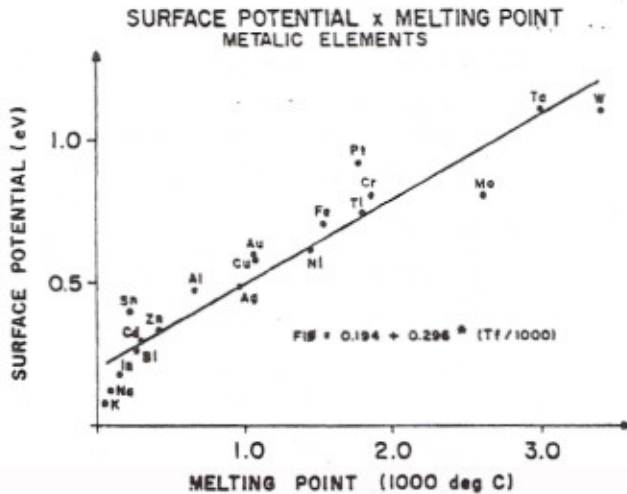


Fig. 3 - Surface potential and melting point correlation.

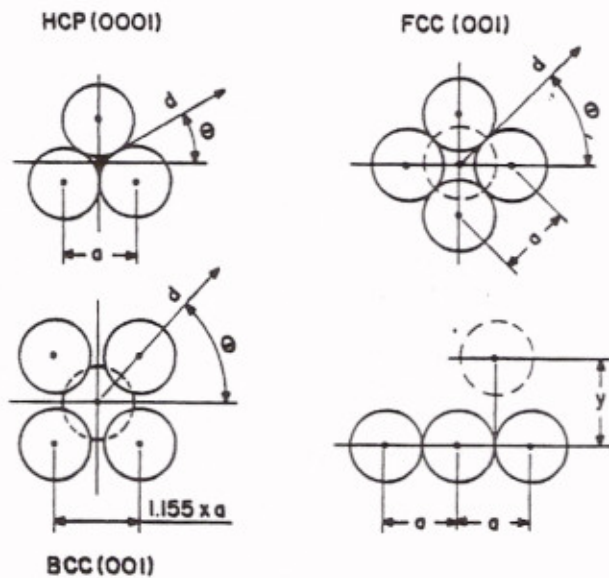


Fig. 4 - Analyzed adsorption sites surface geometries.

Most research in which the surface energy is a key property, is usually related to technological processes such as catalysis, painting, bonding, etc. and have opposed objectives to that of the present work, that is, the search how to increase the adsorption forces.

A strong correlation exists between the surface energy and the melting heat, and between the surface potential and the melting point of materials, as shown in Fig 3, for the surface potential of the metallic elements [2].

Some layered crystalline materials have only "Van der Waals" bonds acting between their layers, and for which surfaces, the surface energy levels are much lower than those of otherwise oriented surfaces.

These "Van der Waals" bonds being function of atoms and molecules polarizabilities are weaker for non polar and low polarizability substrata.

4.2 Surface Structure

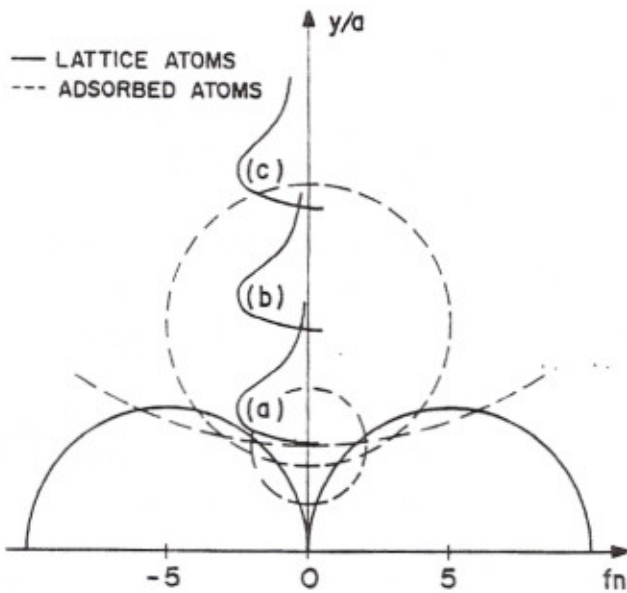
In order to verify the effects of the surface atomic structure on the adsorption forces and on its tangential component, a simplified numerical model was elaborated, using substratum atoms fixed at lattice positions (neglecting the thermal motion).

A "6-12 Lenard Jones" [9] type interaction potential was assumed to act between these substratum atoms and a surface adsorbed atom, and the resultant force was computed by simple summation, what is acceptable for weak interactions.

HCP, FCC, BCC and Tetrahedral solids, without any surface reconstruction (Fig. 4) and three different ratios of the external ("R0"), to the internal ("a") equilibrium distance, have been investigated ($R0/a = 0.7, 1.0$ and 1.4).

From the results, some of which are shown in Fig 5 to 6, it was concluded that, for the same interaction potential parameters:

- The crystal type has a minor influence on the normal component of the adsorption force and so on the adsorption energy.
- The tangential component of the adsorption force and so the energy for moving the adsorbed atom along the surface, are greatly influenced by the surface structure. They are lower for some surface directions and minimized by closed packed (HCP0001) arrangements.



a) $R_0/a = 0.7$ b) $R_0/a = 1.0$
c) $R_0/a = 1.4$

Fig. 5 - Adsorption force normal components.

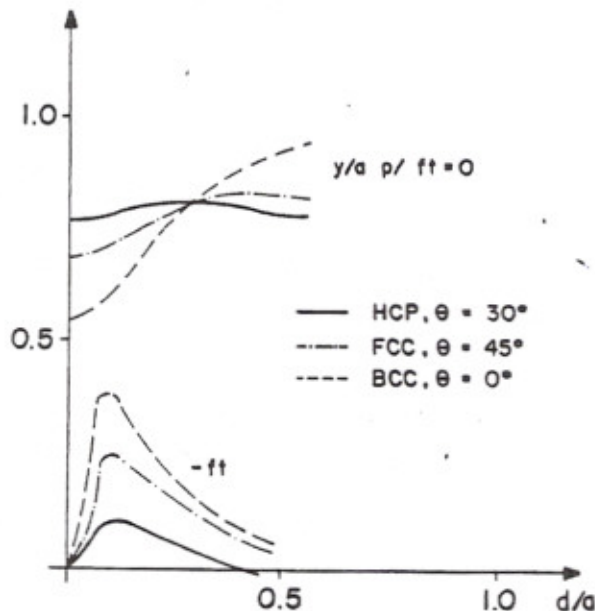


Fig. 6 - Adsorption force tangential component and equilibrium position above surfaces.

5. CONCLUSIONS

It is concluded that, for aerodynamic friction drag reduction purposes, the materials to be chosen for further thin film manufacturing research, shall have, besides obviously a chemical stability in respect to air constituents:

- High atomic and molecular weight.
- Low surface energy, that is: low melting or sublimating temperature, low polarizability, and "Van der Waals" layered structure.
- Closed packed atoms surface structure.

These properties are easy to be found alone, but few materials combine all them, as is the case for some halides and dichalcogenides of heavy transition metals.

Examples are the Bismuth Tri-iodide and the Tungsten Di-selenide, but the most natural candidate for research is the Tungsten Di-sulfide (molibdenite), well known by its solid lubricant properties.

To extend the present single crystal epitaxial grow laboratory technologies, using these low adherent materials [10] [11], to large engineering surface coating processes, undoubting will represent, a formidable molecular engineering defy.

6. BIBLIOGRAPHY

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