

FRICITION DRAG REDUCTION - II (MATERIALS FOR)

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Summary

This paper considers that aerospace vehicle friction drag reductions could result from the use of external surface covering having atomic level smoothness, obtained by crystal grow processes. The dynamics of the gas-solid surface interactions, the adsorption phenomena and the effects of the substrata atomic structure on adsorption forces are discussed in order to identify the most adequate material for such an application.

It is concluded that some heavy transition metal halides and dichalcogenides, with "Van de 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 with zero mean values of the tangential component. However, in many cases, such as He scattering by LiF or Pd 111 (Zangwill, 1988) surface, most gas molecules are elastically scattered resulting in a non-zero mean value.

Also, in the last decades (Lewis, 1976), the micro electronic device development brought with it new manufacturing processes, such as the Molecular Beam Epitaxy, which permit extrapolating for the near future, the possibility to obtain large surfaces with atomic level

smoothness.

The above considerations suggest, as presented in a speculative essay at the XX OSTIV Congress (Galvão, 87), that non-zero slip condition boundary layers and resultant friction drag reductions, could be obtained, although, discrepancies from the zero-slip condition for "engineering" surfaces in dense flows ($KN \ll 1$) have never been verified.

Obtaining such results will be conditional on:

- a) The determination of the materials properties, required to obtain the elastic scattering of air molecules.
- b) The extension of the present single crystal growth laboratory technologies, to large engineering surface coating processes, which represents, a formidable molecular engineering defy.

The benefits to be obtained, not only in terms of increased glider performance but also in low-orbit satellite increased life-times and in aerospace vehicles fuel economies, could be quite remarkable. The present work tries to identify the most adequate materials that fulfill the first (a) condition so that with further research on (b), the predicted drag reductions could be experimentally verified.

2. Dynamic Interactions

Mass effects: Although the dynamic interactions between atoms and molecules and solid surfaces have been extensively studied (Goodman, 1976), it seems to be a rather complex subject, which explains the different theoretical models and some conflicting experimental results found, in the literature.

The classic mechanics models such as "hard cubes", "soft cubes", etc, suppose a zero tangential momentum transfer, and simple and accurate models giving the theoretical computation of the tangential momentum accommodation coefficient, and the corresponding friction drag, are not available.

Elaborate numerical simulations (Tully, 1984) and dissipative quantum phenomena such as, electron-hole pairs, (Lundquist, 1984) are to be considered, if precise results are wanted.

A simple, but partial approach is the use of the old and classic mechanical rigid spheres model (Zangwill, 88), of "Baule", which evaluates the energy accommodation as a function of gas temperature and of the atomic masses involved.

This is the approach used for the computation of the drag and lift forces in satellite aerodynamics (Boechter, 1983), where the gas/solid atomic mass ratio is the preponderant parameter, owing to the values of the interaction energies involved,

Owing to the tangential to normal, and to the translational to rotational momentum transfers of the colliding gas molecules, a low accommodation of the energy, does not imply a low tangential momentum accommodation, but it is a necessary condition for it.

The "Baule" model shows that in order to result in elastic reflections the solid surface atoms must be much heavier than the gas atoms and molecules, and it explains the elastic scattering obtained with light atom

(helium) beams from single crystal surfaces in vacuum.

The effect of the atomic layers beneath the surface is more complex and related to the solid "phonon" characteristics.

An extension of the purely mechanical reasoning already employed, indicates that heavier inner atoms, especially when strongly attached to surface atoms, will contribute to reducing the energy accommodation or phonon excitations.

A final conclusion is that for aerodynamic friction drag reductions purposes, only materials presenting surface atoms heavier than the Nitrogen should be considered and high density materials should be preferred.

Contamination Effects: Another important aspect to be considered in gas-surface interactions is the effect of the presence of adsorbed species on the surface.

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

In all practical applications and at normal atmospheric conditions, the surface contamination by the air constituents, especially of water vapor molecules and also by solid dust particles of all sizes and types, seems unavoidable.

A partial solution to this problem seems to be the reduction of the surface adsorption forces to a minimum.

The reasoning is that if adsorption forces, especially the tangential ones are kept small, the loosely adsorbed species could easily "slip" along the surface with small tangential momentum transfer.

3. Adsorption Forces

Surface Energy: The physical adsorption is a widely studied subject and the key phenomenon for catalysis, painting, bonding and many other technological processes, for which the objective is how to increase the adsorption forces.

These forces, which result from the fact that solid atoms or molecules cohesion energy remains unbalanced at the solid surface are described by the material characteristic known as surface energy or surface potential.

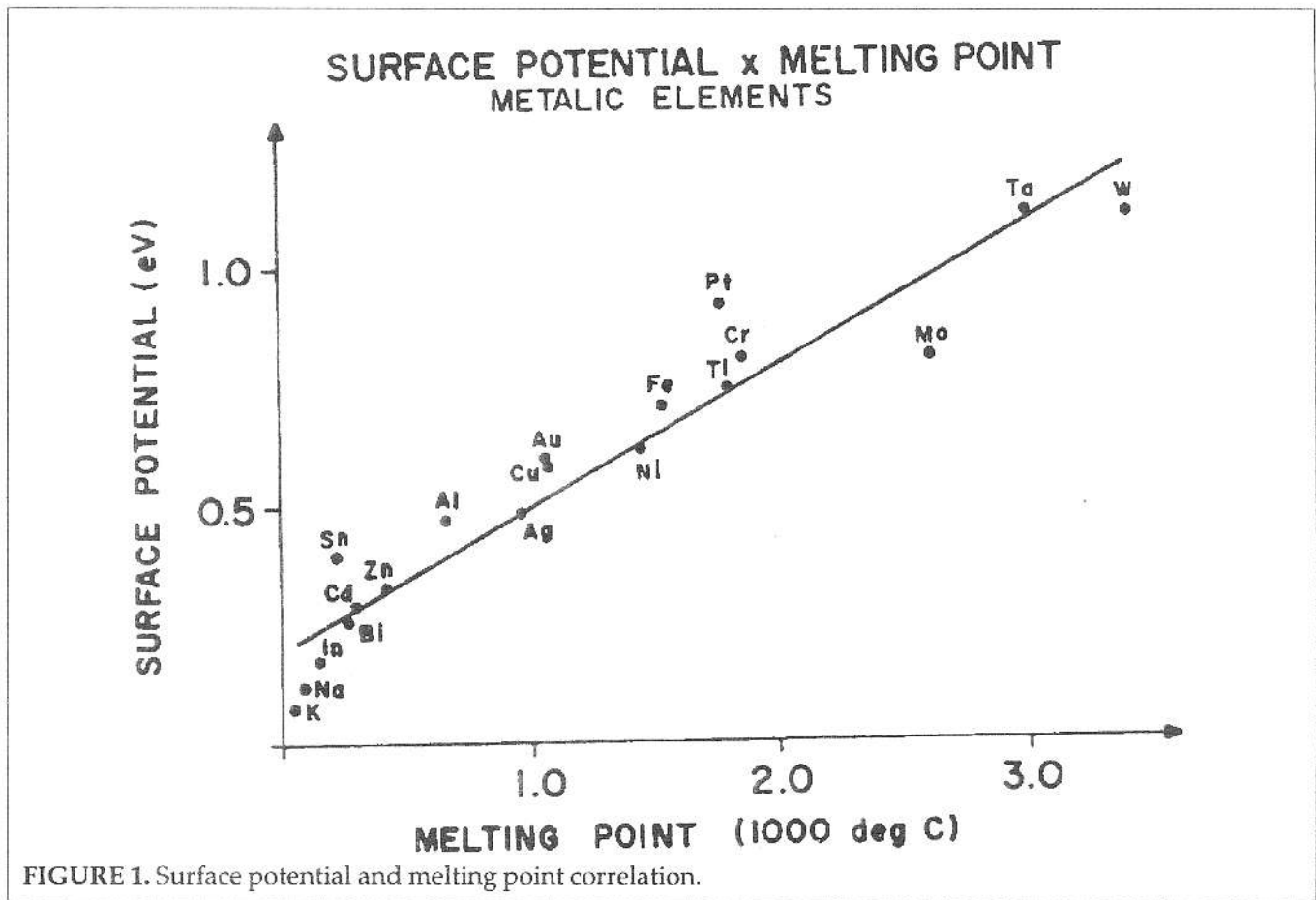
The surface energy can be correlated with the melting heat and the surface potential to the melting point of materials as shown in Fig 1, for the metallic elements.

Materials, may show different values for surface energies, depending on the orientation of the surface being considered and on its atomic structure.

The low energy surfaces are those for which the smallest number of atomic bonds are left "unfilled" or "dangling" and these bonds are of the weak "Hydrogen" or "Van der Waals" types.

In consequence, low-energy surfaces can also be found in materials such as graphite, mica, talc, etc. which have high values of "bulk" or internal energies, but also have layered atomic structures with only weak bonds acting between the layers.

The "Van der Waals" bonds result from electron cloud



asymmetries which can be of three types:

The first type is the purely geometric asymmetry in polar molecules, the second the asymmetry induced in otherwise symmetric atoms and molecules by polar molecules and the third by the instantaneous asymmetry inherent in all electron clouds, that generates the forces known as "dispersion" forces.

The effect of the induced asymmetry is normally small of the two last asymmetries are functions of the atom polarizabilities.

In summary, surface energies and adsorption forces are smaller for "Van der Waals" type surfaces of non polar or low-polarizability substrata.

Surface Structure: In a macro approach, any surface roughness and porosity result in an increase of the surface area and of the adsorption forces, as can be verified in adhesion, catalysis and painting processes.

The single crystal surfaces represent the limit of attainable smoothness, but even they can be quite "rough" to the adsorbed atoms and molecules.

To verify the surface atomic structure effects on adsorption forces, a simplified numerical model has been constructed with the substratum atoms fixed at lattice positions and so neglecting any thermal motion.

The forces between these atoms and a substratum surface adsorbed atom, have been assumed to be derived from a "6-12 Lenard Jones" potential (Ashcroft, 1976) and so computed as:

$$f = 1 / r^7 - 1 / r^{13} \quad (1)$$

with: $f = F \cdot R_0 / 12 \cdot F_{i0}$
 $r = R / R_0$

where F_{i0} and R_0 are the equilibrium potential and radius of the substratum and adsorbed atom interaction and F is the interatomic force at distance R .

The resultant force was computed by simple summation of all the pairwise interaction forces, which is acceptable for weak interactions.

This simplified numerical model was applied to HCP, FCC, BCC and Tetrahedral lattice substrata, without surface reconstruction, and considering three values; 0.7, 1.0 and 1.4, for the ratio between the external/internal atomic equilibrium distances R_0 .

From the results, some of which are shown in Fig 2 to 4, it was concluded that besides the influence of the interaction potential parameters:

- The crystal lattice 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 the energy for moving an adsorbed atom along the surface, are both greatly influenced by the surface structure. They are lower for some surface directions and minimized by closed packed surfaces (HCP0001).

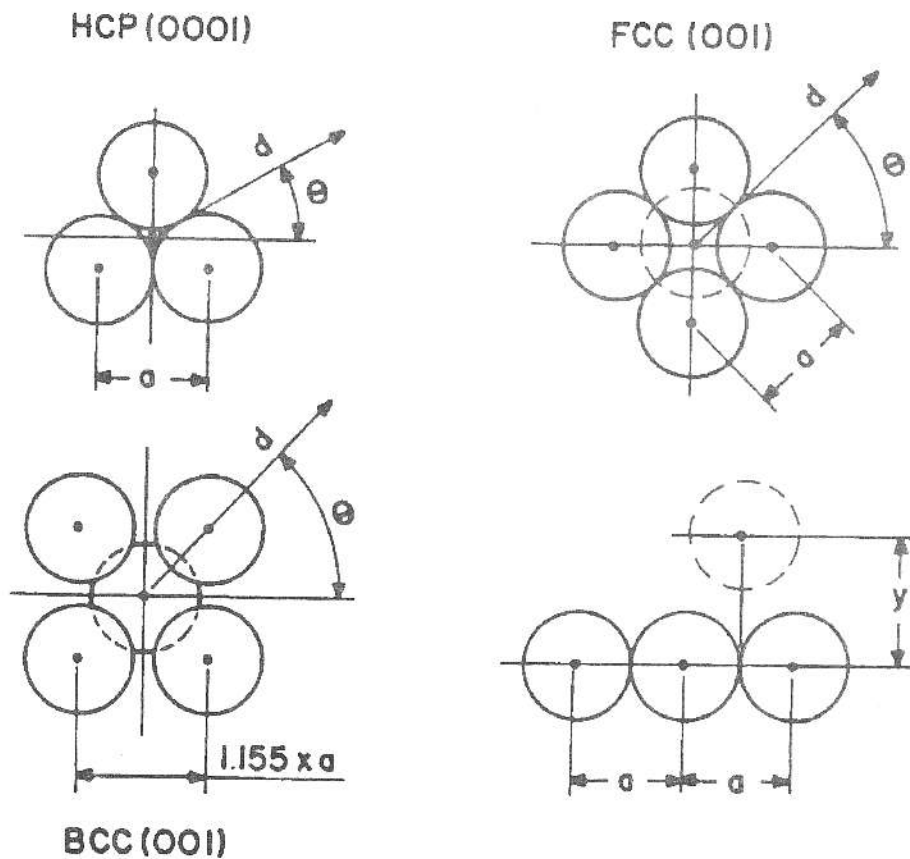


FIGURE 2. Analyzed adsorption sites surface geometries.

4. Conclusions

From the above considerations, it is concluded that the candidate materials for further thin film research to obtain fluid friction drag reductions over single crystal surfaces shall have:

- Heavy surface atoms and high specific mass,
- Low energy surfaces, that is:
 - Low melting or sublimating temperature.
 - Non-polar molecules and low polarizability.
 - "Van der Waals" layered structure.
- Closed packed atom surface structure.

In addition to the above physical characteristics, the materials must have a chemical stability in respect to air constituents.

These properties are easy to be found singly, but few materials present all them together, as is the case of the halogenides and di-chalcogenides of the heavy transition metals with "Van der Waals" layered structure (Wells, 1962).

Examples are the Bismuth tri-iodide and the Tungsten

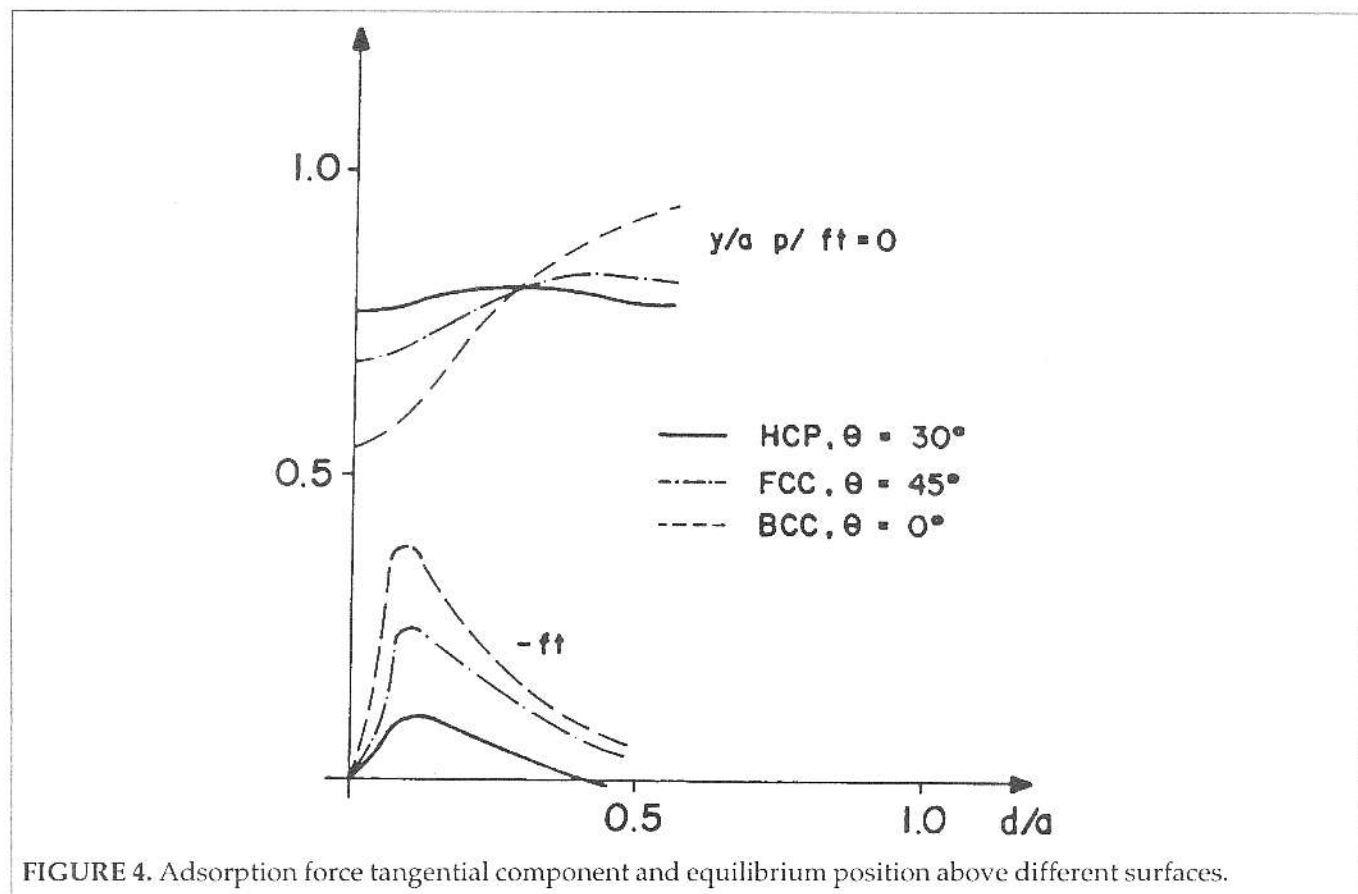
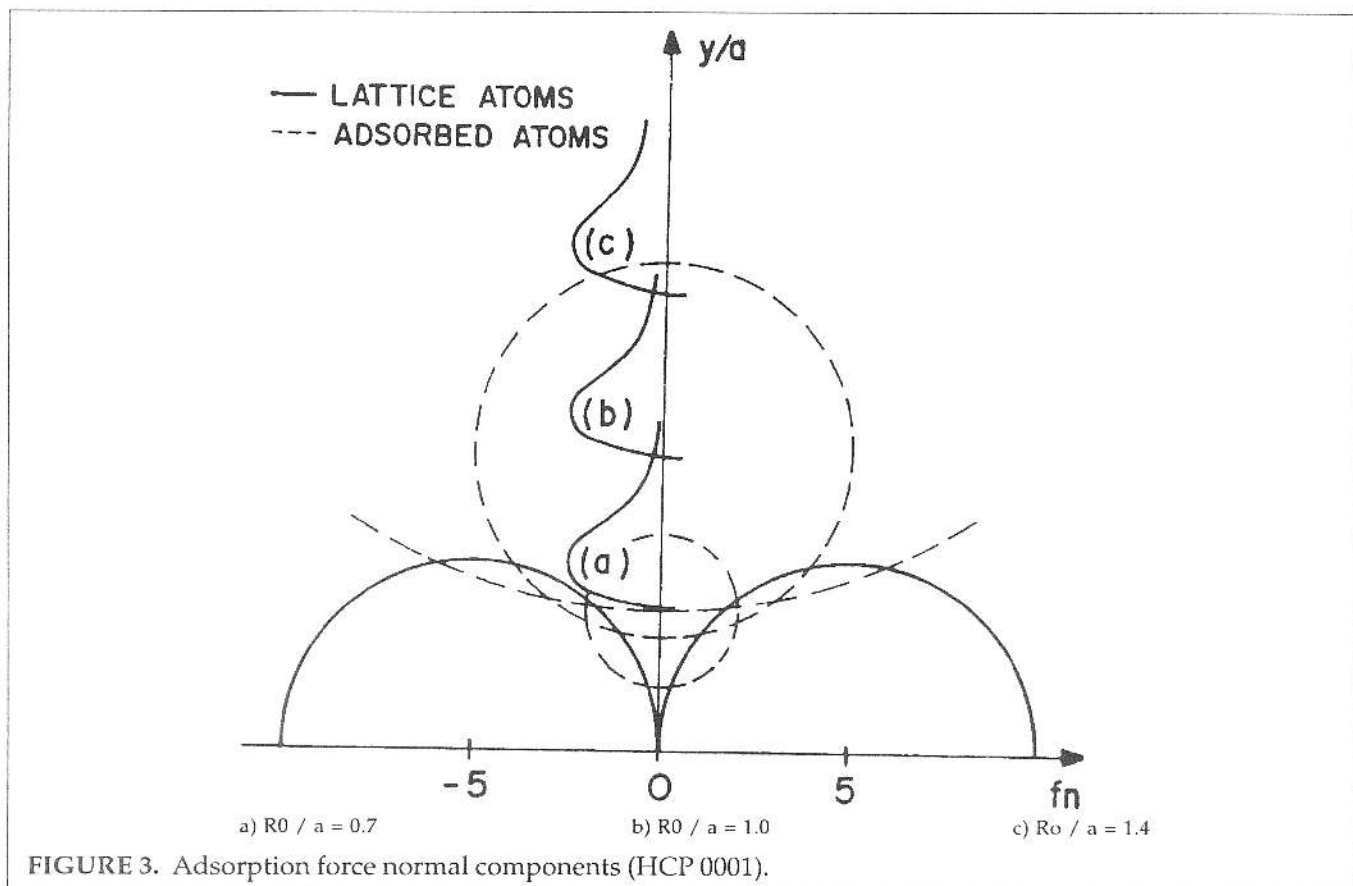
Di-Selenide, but one of the most interesting is the Molybdenum Di-sulfide, which is a natural mineral (Molibdenite), and a well known solid lubricant.

Covering films made of such materials (Ueno, 1990 and Jager, 1991) will give to our presently immaculate white gliders, the grey-black colour of a B-2 stealth bomber..., but also of the best soaring birds!

Since a 50% reduction in friction drag, is equivalent in high speeds, to having a 30% of gross weight ballast, and still present a climb advantage in thermals, who will care about color?

5. References

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