

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:

- The determination of the thin film material properties, required to obtain the elastic scattering of air molecules.
- 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.

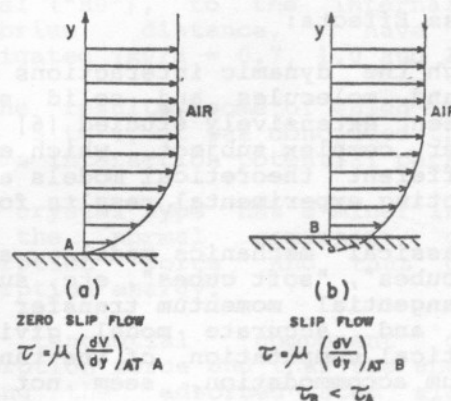
For elongated and "streamlined" bodies such as airplanes, the friction drag can be responsible, at cruising speed conditions, for the major part (around 60%) of the total drag and so of the fuel consumption.

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.



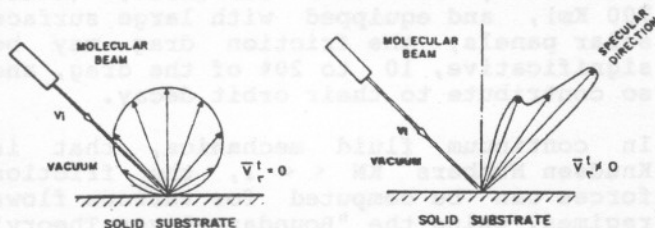
a) zero slip flow b) flow with slip

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 a 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 does not imply 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 heavier than the gas atoms, and molecules, and it explains elastic scattering results obtained in vacuum, for 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 substrate.

An extension of the previous mechanical reasoning, indicates that heavier inner atoms, in particular 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 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 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

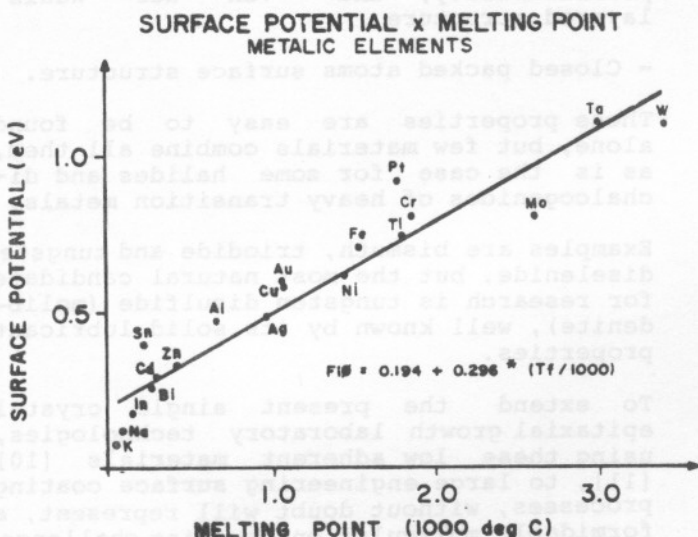


Fig. 3 - Surface potential and melting point correlation.

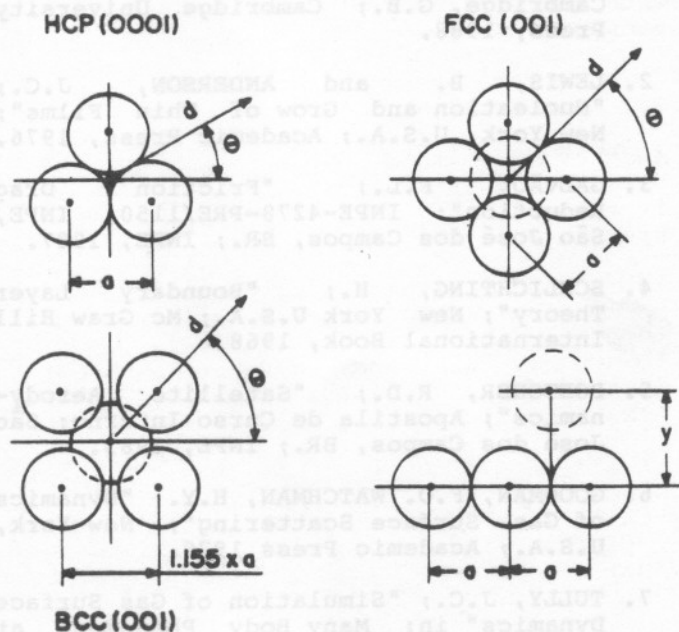


Fig. 4 - Analyzed adsorption sites surface geometries.

Research in which the surface energy is a key property, is most related to technological processes such as catalysis, painting, bonding, etc. and have opposed objectives to that of the present work, that is, the search of 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 substrate atoms fixed at lattice positions (neglecting the thermal motion).

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

HCP, FCC, BCC and thetetraedral 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 thus on the adsorption energy.
- The tangential component of the adsorption force and thus 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.

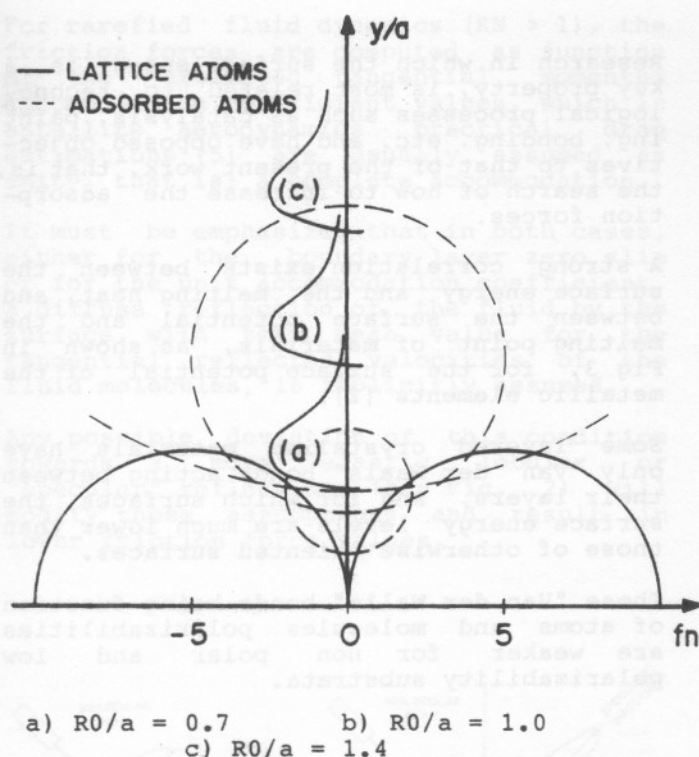


Fig. 5 - Adsorption force normal components.

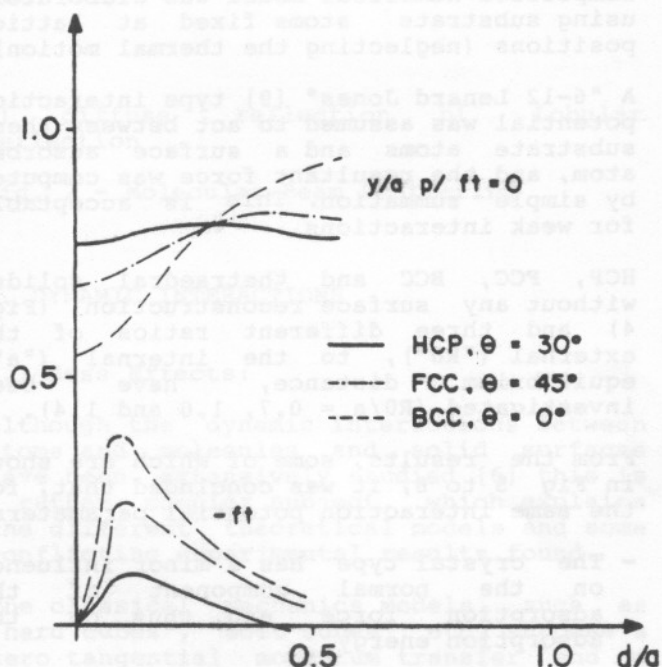


Fig. 6 - Adsorption force tangential component and equilibrium position above surfaces.

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 with 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 bismuth, triiodide and tungsten diselenide, but the most natural candidate for research is tungsten disulfide (molibdenite), well known by its solid lubricant properties.

To extend the present single crystal epitaxial growth laboratory technologies, using these low adherent materials [10] [11], to large engineering surface coating processes, without doubt will represent, a formidable molecular engineering challenge.

6. BIBLIOGRAPHY

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RESUMO

O níquel e suas ligas se destacam dentro os metais refratários pelo seu alto ponto de fusão (1455°C), pelas suas ótimas propriedades mecânicas e resistência à oxidação. Porém sua alta velocidade de oxidação em temperaturas acima de 500°C, limita a sua condição de trabalho. Este problema pode ser controlado com a adição de elementos de liga ou com um revestimento superficial que impede a infiltração do oxigênio. Neste trabalho são apresentados: 1) a preparação do revestimento ("coating") pela formação de uma liga ("alloy") composta de pó metálico (Fe, Cr, Si) e carbono, de tipo celulose (CMC) como plastificante, aplicada ao substrato por imersão sendo então curada a uma temperatura de 1500°C durante 1 hora em atmosfera inerte (nitro); 2) as caracterizações do revestimento através de análises microestrutural, microscopia eletrônica de varredura e raio-X; 3) Testes de qualidade como teste de tocha e teste de oxidação cíclica lenta, visando aplicações até 1500°C.

1. INTRODUÇÃO

A importância tecnológica dos metais refratários deriva de seu alto ponto de fusão (1455°C), tornando-os capazes de serem usados em temperaturas mais altas que as que os materiais em outros materiais, como superliga a base de níquel (Ni) e cobalto (Co).

Infelizmente, o ponto de fusão por si só não é suficiente para indicar um metal como de uso de engenharia de materiais em altas temperaturas. Por exemplo as temperaturas de interesse, até 5, acima de cerca de 1500°C, o molibdeno (Mo) oxidado forma MoO₃, tungstênio, o níquel (Ni) oxidado forma NiO e o tántalo (Ta) oxidado forma Ta₂O₅. Com as muitas aplicações de ligas metálicas refratárias o ambiente é oxidante e a degradação ambiental é uma desvantagem para aplicação desses materiais.

Dentre os metais refratários o Ni, Fe, Mo e W têm recebido maior atenção da comunidade metalúrgica. As ligas de Ni ligadas a maior parte de estudo, porque o Ni é caracterizado por sua baixa massa específica, pequena seção transversal de absorção de nêutrons e alta temperatura crítica super-

condutora. Além das suas baixas perdas de fusão, condutividade térmica e módulo de elasticidade, elas podem ser visto na tabela 1. Segundo Savat [3].

R.A. Perkins e Gerald S. Meier [1] em um trabalho recente, 1988, concluem que, apesar de muitos anos de esforço, pesquisadores foram incapazes de desenvolver uma liga de Ni para aplicações em alta temperatura com habilidade para formar uma película de óxido protetora. Os "coatings" têm sido considerados para fornecer proteção à superfície do Ni e suas ligas.

Numerosas técnicas e combinações de técnicas são usadas na fabricação de revestimentos de proteção. Alguns revestimentos mais avançados são aplicados por técnicas de deposição de vapor químico, deposição por hidrogenação, deposição por sinterização e deposição, e infiltração dos poros.

O "coating" a base de silício é considerado como a melhor material para a proteção das ligas de Ni. Os "coatings" de silício de Ni molibdeno (Ni-Cr) e Fe-Ni desenvolvidos por Trimmer e Saxe [1] em 1965, têm sido usados há décadas nos motores a jato. Em 1968, Trimmer e Saxe [2] apresentaram os estudos de otimização das composições, anteriormente desenvolvidas, chegando à conclusão que Si-20Cr-10Fe apresenta o melhor ponto de partida para otimização para proteção à oxidação em altas temperaturas.

Os estudos de "coating" resistentes à oxidação para proteção de ligas de Ni foram revisados recentemente, 1988, por C. N. Parker [4].

Este trabalho tem por objetivo a produção de um "coating" a base de Si-AlCr 10% em bruto sobre o Ni e posterior caracterização visando eficiência, praticidade e aplicação para futuras aplicações em temperaturas superiores a 1500°C.