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This paper considers that aerospace vehicles friction drag reduction could result from the use of external surfaces with atomic level smoothness, obtained by epitaxial grow processes. The adsorption phenomena, the effects of the substratum atomic structure on adsorption forces and the dynamics of the gas-solid surface interactions are discussed in order to identify the adequate material properties 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.

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MATERIALS FOR AEROSPACE VEHICLES FRICTION DRAG REDUCTION SURFACES

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SUMMARY

This paper considers that aerospace vehicles friction drag reduction could result from the use of external surfaces with atomic level smoothness, obtained by epitaxial grow processes. The adsorption phenomena, the effects of the substratum atomic structure on adsorption forces and the dynamics of the gas-solid surface interactions are discussed in order to identify the adequate material properties 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.

INTRODUCTION

In the search for new friction drag reduction methods, it seems interesting to investigate the physical phenomena governing the momentum transfers occurring at the fluid/solid interface, since from them result all the fluid dynamic forces acting on a body, including those forces known as pressure, induced and friction drag.

In fluid mechanics, the tangential molecular momentum transfer, which originates the friction drag, is implicitly assumed as being a total one, either by the boundary layer "no-slip" condition used in dense flows or, according to flow "Knudsen Number", by the unity value of the accommodation coefficient normally used in rarefied flows.

While for "engineering" surfaces the value of the tangential accommodation coefficient has been subjected to some discussion, as in satellite aerodynamics, and non zero slip values are used in "transition flows", discrepancies from the zero-slip condition in dense flows were never verified in the experimental results.

In the last decades however, the micro electronic device technology brought with it new manufacturing processes (Lewis, 1978), such as the "Molecular Beam Epitaxy" and others, which permit to extrapolate for the near future the possibility of obtaining large surfaces with atomic level smoothness.

From the first experiments made to verify some gas kinetic theory assumptions (Loeb, 1961), a largely used tool has been the study of the scattering of molecular beams produced by single crystal surfaces, in vacuum.

Most experimental results showed scattered patterns having a "Maxwellian" or "sinus law" velocity distributions with zero mean values of the tangential component, in a good agreement with the tangential momentum total accommodation assumption.

However, in some cases, for instance in the scattering of helium molecular beams by alkali halides (i.e. Li F) single-crystal surfaces , a non negligible amount of the gas molecules is elastically scattered with specular or diffracted velocity distributions which have non zero mean value for their tangential component (Goodman, 1976).

Such results show that over single-crystal surfaces, it may be possible to have either boundary layers with non zero slip conditions, in liquid and dense gas flows, or low tangential accommodation in rarefied gas flows.

These considerations open new possibilities of obtaining friction drag reductions (Galvão, 87) in aerospace and waterborne vehicles such as satellites, airplanes, boats etc., which possibilities, will evidently be conditioned to:

a) the determination of the material properties required to obtain elastic scattering of air and water molecules from single crystal surfaces.

b) the development of manufacturing methods to obtain an atomic level smoothness in substantial percentage of large surface coverings made with such materials.

The study of that first condition is the objective of the present work which, in assuming single crystal surface topology, investigates:

- The parameters governing the fluid atoms and molecules physical adsorption by solid surfaces and the surface structure effects on the tangential component of the adsorption force (static interactions).

- The parameters governing the collision between fluid and solid surface molecules and atoms (dynamic interactions).

STATIC INTERACTIONS

Surface Energy. The physical adsorption is a widely studied subject with many applications in catalysis, painting, bonding and many others technological processes, all of them having opposed objectives to the present work, that is, they search how to increase the adsorption forces.

The main solid material characteristics governing these phenomena is the surface energy or surface potential which result from the fact that solid atoms or molecules cohesion energy remain unbalanced at the solid surface.

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 1, for the surface potential of the metallic elements.

SURFACE POTENTIAL x MELTING POINT
METALIC ELEMENTS
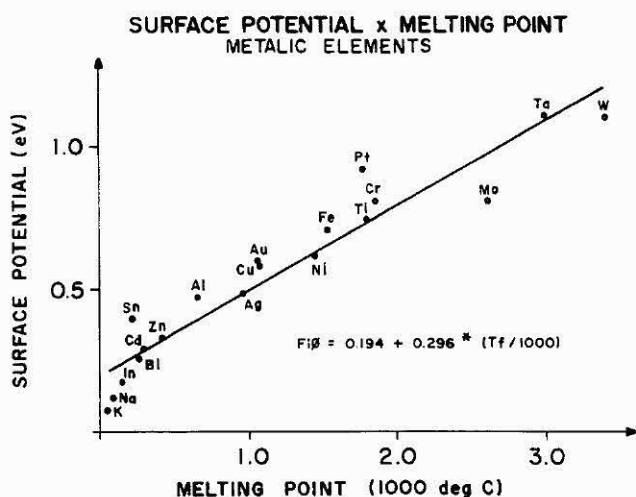
Fiø = 0.194 + 0.296 * (Tf / 1000)

Fig. 1 Surface potential and melting point correlation.

For the same material however, we may find different values for surface energies, depending on the orientation of the surface being considered and on the material atomic structure.

Low energy surfaces shall leave unfilled the smallest number of atomic bonds (referred as "dangling bonds") and preferably shall "cut" through the weaker ones.

Since the weaker atomic bonds are those of the "Van der Waals" and "Hydrogen" type, low surface energy values occur in materials such as graphite, mica, talc, etc., which have layered atomic structures, with only these bond types acting between the layers.

Unlike hydrogen bonds, which present nearly constant intensities, the "Van der Waals" bonds can vary considerably according to the molecule or atom types which participate in the bonding and they can be decomposed in three components, all them resulting from electron cloud asymmetries:

A first component is due to any geometrical molecular asymmetry (in polar molecules), a second to the asymmetry induced in atoms and symmetric molecules by polar molecules and a third by the instantaneous asymmetry ("dispersion" forces) inherent to all atomic electron clouds.

The second and third components are function of the atom and molecule polarizability, the second being much smaller than the two others and the "dispersion" component depending also on the number of electrons in atom outer shell (Kondratiev, 1967).

So surface energies shall be smaller for "Van der Waals" type surfaces of non polar substrata having low polarizabilities.

Suface Structure. Concerning the effects of the surface structure on adsorption forces, in a macro approach, the increase in surface area created by roughness and porosity result in increased forces, as verified from adhesion, catalysis and painting processes.

Although single crystal surfaces provide the maximum possible "macro" smoothness, they can be quite "rough" in atomic scale to the adsorbed atoms and molecules.

In order to study the effects of the surface atomic structure on the adsorption forces, in special on its tangential component, a simplified numerical model has been constructed.

In this model the substratum atoms were supposed to be fixed at lattice positions (neglecting thermal motion) and the forces between these atoms and a substratum surface adsorbed atom, have been assumed to be derived from a "6-12 Lenard Jones" potential (Ashkroft, 1976) and so computed as:

$$f = 1/r7 - 1/r13 \qquad (1)$$

with: $f = F \cdot RO / 12 \cdot FiO$ and $r = R / RO$

where FiO and RO are the equilibrium potential and radius of the substratum and adsorbed atom interaction and F 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 Thetraedral lattice substrata and for three different values: 0.7, 1.0 and 1.4 for the ratio of the external to the internal (half lattice constant) equilibrium distances .

From the results, some of which are shown in Fig 2 to 4, it was concluded that:

- The crystal lattice type has a minor influence on the normal component of the adsorption force and so on the adsorption energy, which depends mainly on the atomic potential parameters values being proportional to FiO/RO.

- That is not the case for the tangential component of the adsorption force and hence for the translatioonal energy of a surface adsorbed atom, which besides depending on adsorption potential parameters are also greatly influenced by the surface structure.

- These tangential forces and energies are lower for some surface privileged directions and are minimized by closed packed surface arrangements such as the HCP (0001).
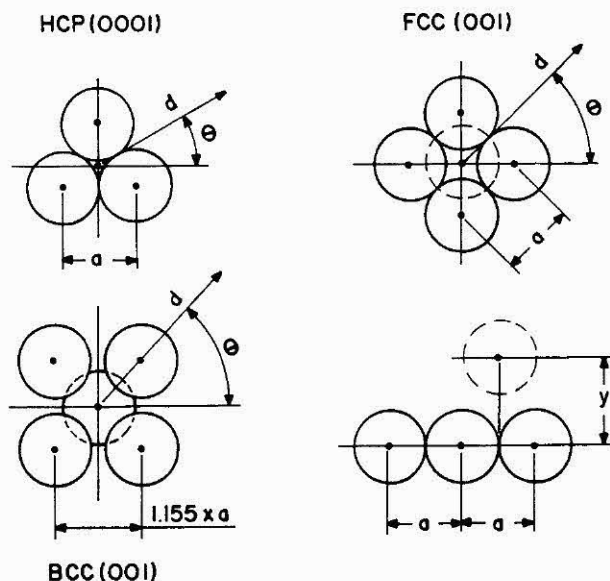

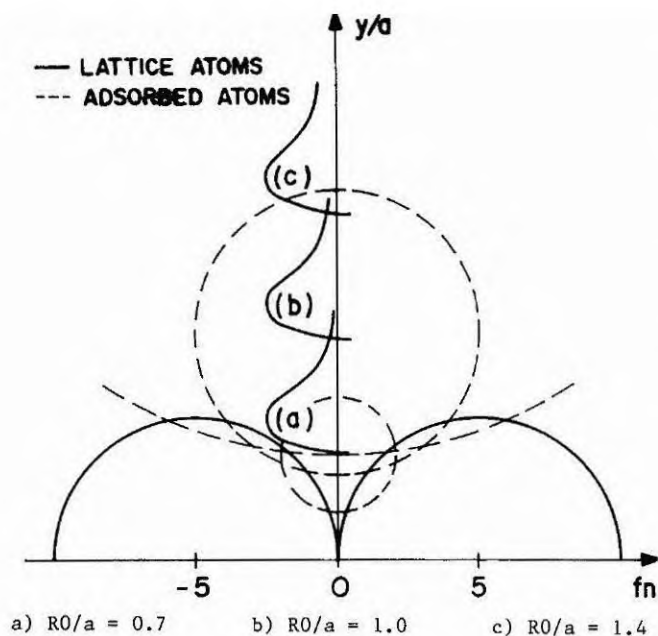Fig. 2 Analysed adsorption sites surface geometries.

a) R0/a = 0.7   b) R0/a = 1.0   c) R0/a = 1.4

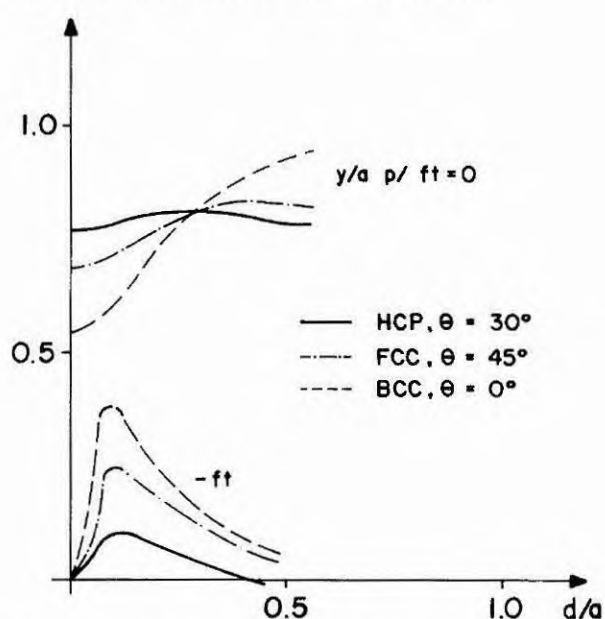Fig. 3 Adsorption force normal components.

Fig. 4 Adsorption force tangential component and equilibrium position above different surfaces.

DYNAMIC INTERACTIONS

Although the dynamic interactions have been extensively studied (Goodman, 1976), they seem to be rather complex and even for simple cases a completly representative theoretical model was not available in the searched literature.

The existing theoretical classical mechanics models such as "hard cubes", "soft cubes" etc, suppose a zero tangential momentum transfer and even some complex and complete numerical simulations (Tully, 1984) do not take into account the dissipative quantum phenomena (Lundquist, 1984) such as substratum phonon creations.

It seems that the only usefull results, are those from the classic "Baule" rigid spheres mechanical model for gas solid surface interaction, which allow the evaluation of the energy accommodation coefficient as function of gas temperature and gas and solid atomic masses.

This Baule model is used in satellite aerodynamics for the accommodation coefficient evaluation and the drag and lift forces computation (Boechter, 1983), for which the gas/solid atomic mass ratio becomes the preponderant parameter due to the high values of the interaction energies involved.

Although low energy accommodation coefficient values do not imply in a low tangential momentum accommodation, this is a necessary condition for it, which means that, at least for gas/solid interactions, the surface atomic and molecular weights must be much higher than gas ones in order to increase the elastic reflections.

CONCLUSIONS

From the fluid/solid surface interaction factors considered, it is concluded that the material charachteristics that could result in possible fluid friction drag reductions for single crystal surfaces are:

- Low melting or sublimating temperature.

- Non polar molecules and low polarizability.

- Crystalline structure with close packed atoms layered arrangement with "Van der Waals" bonding between layers.

- High atomic and molecular weight.

In addition to the above physical characteristics, the considered materials must be also obviously, neither soluble nor chemically reactive in respect to the fluid they will be in contact to.

These properties are found individually in many materials such as: Graphite (layered structure), "Teflon" (chemical inertia and low polarizability), Cadmium (high density, low melting point and close packed surface), but few present all them together.

Some halides and di-chalcogenides of heavy transition metals which crystalize with "Van der Waals" layered structure (Wells, 1962) such as the Bismuth Tri-iodide and the Molybdenum Di-sulfide (has also a remarkable low solid friction coefficient), represent however a good starting point for further research.

To extend the present single crystal epitaxial grow laboratory technologies, using these low adherent materials (Ueno, 1990), to large engineering surface coating processes, undoubtly will represent, a remarkable molecular engineering feat.

The benefits to be eventually obtained, in terms of aerospace vehicle fuel economies and of low orbit satellite increased life-times, could be however, not less remarkable.

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