Influence of Different Environment on the Tribological Behavior of Molybdenum Disulfide MoS₂

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Abstract:- Plastic materials are more and more important in our life. This article measure the thermal properties of some typical plastics materials by using the TMA Q400 machine. By comparision of their results and their chemical formulas will show their properties.

The tribological properties of molybdenite or molybdenum disulphide MoS₂ depend on the relative humidity of gases surrounding the tribocontact. In high vacuum environments and in inert gases, the friction coefficient μ of molybdenum disulphide MoS₂ is very low about μ=0,02 and in humid environments, the friction coefficient increases to μ = 0,18.

The objective of this study is to present the experimental results of the tribological properties of molybdenum disulfide MoS₂ against steel XC48 in different gaseous environments (in high vacuum and ambient air). We calculate the potential energy between the gaseous molecules and the surface of adsorption or between these adsorbed gaseous molecules. We also try to estimate the interactions between the adsorbed gaseous molecules of the gap between the two consecutive layers of the crystal molybdenum disulfide MoS₂. We discuss the effect of these interactions on the tribological charactistics of molybdenite MoS₂.

Keywords:- Molybdenum Disulphide, Water Vapor, Polarisation, Ionization Energy, Lubrification, Friction Coefficient.

I. INTRODUCTION

Molybdenum disulfide MoS₂ crystal is a hexagonal structure. It is a solid lubricant lamellar structure of alternating layers: layer of sulfur / molybdenum layer / layer of sulfur ... layer of sulfur / molybdenum layer / layer of sulfur ... (S / Mo / S ... S / Mo / S ...). Its low friction coefficient μ = 0.02 obtained in high vacuum around tribocontact is due to the weak bonds Van der Waals [1-15] between two layers of sulfur. However, this low coefficient of friction can vary and increase to μ = 0.18 in air ambient around the tribocontact [1-15].

In the previous time, we did not attribute the variation of friction coefficient molybdenum disulfide MoS₂ in the environment around tribocontact [19]. Since 1976, it demonstrates with the notion of "time stop effect" that there is an influence of water vapor, gases or other contamination on the friction coefficient. In this paper, we present the experimental results obtained in four tribological different gas environments. Then we discuss the reasons which change the friction coefficient in the different gaseous environments.

II. DESCRIPTION OF EXPERIMENTAL TESTS

Tribological tests were done by using one pin-on-disc type tribometer as shown in the figure 1. The pin is hemispherical shape with diameter of 5 mm and length of 15 mm. The disc diameter is 70 mm which is covered by a thin layer of molybdenum disulphide MoS₂. Both of them are made of steel XC 48 and they are localised in the chamber of tribometer.

The different gaseous types used for the experimental tests such as dry ambient air. The temperature is nearly stable about 25° C. The relative sliding speed is 0,4 m/s. The normal load N is 4,625 N applied with the mass on the arm carrying the pin.

To prepare the experimental in high vacuum, the air of the closed chamber is evacuated by a system of pumps. A primary pump can descend to a pressure of 10⁻¹ Pa. A second turbo pump continues descend down to 10⁻⁵ Pa in 24 hours. Once the high vacuum reached, we can start the friction tests in high vacuum.

The friction force is recorded by a gauge. The various sensors are connected to a central acquisition of multichannel data. The analog signal is amplified and converted by a conditioner Labview 7.1.
III. RESULTS AND DISCUSSIONS

All the gaseous contamination in the molybdenum disulfide produced an increase in friction coefficient compared with the value obtained in high vacuum. Indeed, it has been shown experimentally in several publications [1,15].

The contamination by the vapors is probably inherently an impact on the structure of molybdenum disulfide MoS$_2$ and produces an increase of friction coefficient rather than the one in high vacuum. In fact, it has been demonstrated experimentally in a wide range of publications reported that it increases the friction coefficient when the two consecutive layers of molybdenum disulfide sliding parallel with the basal planes of the crystallites.

For each experiment, we must change the new pin and the new disc.

A. Tribological behavior of molybdenum disulfide in high vacuum ($10^{-5}$ Pa)

Once the contact pin of steel / molybdenum disulfide / steel disc is established is placed, the chamber is pumped by a primary pump for an hour until the residual pressure $P = 10^{-3}$ Pa and then the secondary pump descends the residual pressure $10^{-5}$ Pa in 24 hours.

Our test of the tribological contact steel / MoS$_2$ / steel carried out in high vacuum ($P = 10^{-5}$ Pa) lead to a friction coefficient $\mu = 0.018$ in steady state (Figure 2).

B. Tribological behavior of molybdenum disulfide in ambient air

Under the influence of a mixture of several gases such as ambient air, the coefficient of friction is not stable (Figure 3). It varies between the value $\mu = 0.18$ at the start of the test and $\mu = 0.12$ at steady state and depends on the concentration or percentage of the gases in the mixture.

IV. DISCUSSION

The molybdenum disulphide is gray-black in color and the density is 4800-5000 kg / m$^3$. It is easily transmitted to another surface. If it attaches to a surface and it is difficult to wash. Transfer is easy for all surfaces because it easily sticks to surfaces. In reality, there are two forms: hexagonal and rhombohedral. We can also list certain physical properties; the most important ones are:

- Melting point: around 1700 °C under atmospheric pressure
- Molecular mass: 160.08 g / mol
- Hardness (basic planes): 1-1.5 Moh scale
- Hardness (crystal edges) 7-8 Moh scale
- Magnetic properties: diamagnetic
- Sublimation temperature: 1050 °C under high vacuum
- Dissociation temperature: 1370 °C
Some authors use the inorganic fullerene of molybdenum disulfide in oil to improve its tribological characteristics and its viscosity. The two families of molybdenum disulfide, the rhombohedral structure (rh) and the hexagonal structure (hcp), on which the research work is based, will be presented.

Figure 4 shows the crystal resemblances between the rhombohedral (rh) and hexagonal (hcp) structure. The distances between sheets are different. It is 1.23 nm in the hexagonal structure and 0.615 nm in the rhombohedral structure (Figure 4).

![Fig 4: The two main structures of molybdenum disulfide MoS₂: hexagonal (hcp) and rhombohedral (rh)](image)

Molybdenum disulfide has been widely studied for a long time. The studies relate to its physical, chemical character and also on its tribological behavior.

We study the electronic configurations of molybdenum atoms and sulfur atoms, so that we can find the optimal combination.

- The electronic configuration of molybdenum is: 
  1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰ 4s² 4p⁶ 5s¹ 4d⁵

- The electronic sulfur configuration is: 
  1s² 2s² 2p⁶ 3s² 3p⁴

If we arrange valence electrons in the 5p orbit 5s 4d for the molybdenum atom and 3s, 3p for the sulfur atom, we have arrangements of the electrons in the orbitals and the overlap of the orbitals (figure 5):

![Fig 5: MoS₂ molecular orbitals structures](image)

In order to stabilize the MoS₂ molecules, the molybdenum and the sulfur are hybridized to sd^4 and the structure of MoS₂ obtained is a hexagonal structure. The crystal structure of natural molybdenite (molybdenum disulfide) is hexagonal, with the basic coordination unit of molybdenum disulfide MoS₂ is a trigonal prism: the molybdenum Mo atom is located in the center of the right trigonal prism and itself is surrounded by six sulfur atoms at the vertices of this prism and each sulfur atom is equidistant from three molybdenum atoms. The crystal structure of molybdenum disulphide MoS₂ can be considered as a stack of XMX macromolecules whose valences are all saturated. Because of the special structure of the molybdenum disulphide MoS₂ due to the sd4p hybridization of the Mo and S atoms, we have a hexagonal shape (Figure 5) which is symmetrical and self-balanced.

The consecutive sulfur layers are linked together by fairly weak forces, while the bonds between molybdenum and sulfur in each layer are covalent and under the influence of the different conditions such as ambient air, in high vacuum, it will be influenced the friction coefficients of molybdenite MoS₂. It has a very large anisotropy of the crystal and an easy cleavage parallel to the basal plane.

V. CONCLUSION

Our tests conducted on the tribological couple acier/MoS₂/acier in high vacuum (P = 10⁻⁵ Pa), and in ambient air that illustrate the influence of environment around the tribo-contact tribological behavior of MoS₂:

- Tests under high vacuum demonstrate clearly the intrinsic nature of self-lubricating molybdenum disulfide \( \mu = 0.02 \). Disulfide behaves almost as well as a lubricant fluid.

- The tests carried out under ambient air clearly show the influence of the properties of different gases on the tribological molybdenum disulfide MoS₂.

- It is interesting to perform tribological tests in mixtures of gases (argon + oxygen), (nitrogen + oxygen) ..., (nitrogen + oxygen + water vapor) to determine the partial pressures at critical transition (low friction / friction severe).

REFERENCES

