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# Experimental and theoretical investigations of friction properties of graphite intercalated compounds.

J.L.Mansot<sup>1,2\*</sup>, K. Delbé<sup>3</sup>, P. Baranek<sup>4</sup>, P. Thomas<sup>1</sup>, F. Boucher<sup>5</sup>, F. Vangelisti<sup>6</sup>, D. Billaud<sup>6</sup>.

<sup>1)</sup> Groupe de Technologie des Surfaces et Interfaces (GTSI EA 2432) Université des Antilles et de la Guyane,

<sup>2)</sup> Centre Commun de Caractérisation des Matériaux des Antilles et de la Guyane (C<sup>3</sup>MAG), Université des Antilles et de la Guyane Campus de Fouillole, BP 250 97157 Pointe à Pitre, Guadeloupe, F.W.I

<sup>3)</sup> Laboratoire Génie de Production, EA 1905, École Nationale d'Ingénieurs de Tarbes, BP 1629, 65016, Tarbes Cédex

<sup>4)</sup> EDF - R&D, Department MMC and MAI, Avenue des Renardières, Les Renardières, 77818 Moret sur Loing Cedex

<sup>5)</sup> Laboratoire de Chimie des Solides, Institut des Matériaux Jean Rouxel, UMR 6502 CNRS-Université de Nantes, 2 rue de la Houssinière, BP 32229, 44322, Nantes Cédex 3, France

<sup>6)</sup> Institut Jean Lamour, UMR CNRS 7555, Faculté des Sciences, Université Henri Poincaré Nancy I, BP 239, 54506 Vandœuvre-Lès-Nancy Cédex, France

\*Corresponding author [jean-louis.mansot@univ-ag.fr](mailto:jean-louis.mansot@univ-ag.fr)

## 1. Introduction

It is classically admitted that the good friction properties of lamellar compounds are strongly related to their anisotropic structure and especially to the existence of weak interlayer interactions through the van der Waals gap separating the basal layers [1]. As it is also known, the presence of the van der Waals gap in the structure of lamellar compounds will allow lot of chemical species to be intercalated in the structure leading both to the expansion of structure parameters and inter layer interactions modifications [2]. The present work is concerned with the experimental and theoretical study of friction properties of Graphite Intercalated Compounds (GICs) in order to better understand the tribological lamellar compounds. In order to modulate the interlayer interactions, two types of intercalated species were used, electrophilic species ( $\text{AlCl}_3$ ,  $\text{FeCl}_3$ ,  $\text{SbCl}_5$ ) and nucleophilic species (Li, K, Rb).

## 2. Experimental and theoretical method

Friction properties were studied using a reciprocal sphere/plane (AISI52100/AISI52100) tribometer under pure argon atmosphere. The electronic properties and interlayer interactions were investigated using ab initio band structure calculations based on DFT theory [3].

## 3. Results and discussion

Tribological results collected on the various GICs are presented in figure 1.

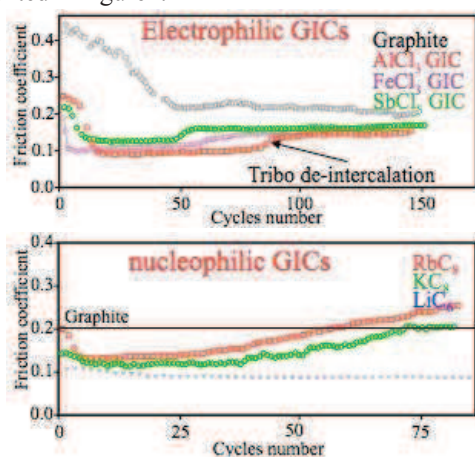


Figure 1: Evolution of friction coefficients as a function of cycles number for the two GICs families.

As it can be seen, the various GICs compounds present

better intrinsic friction coefficient (measured in the early stage of friction tests) than graphite. Most of the compounds presents a de-intercalation process during sliding leading to an increase of the friction coefficient as a function of cycles number.

The figure 2 presents the evolution of the intrinsic friction coefficient as a function of the calculated interlayer interaction intensities.

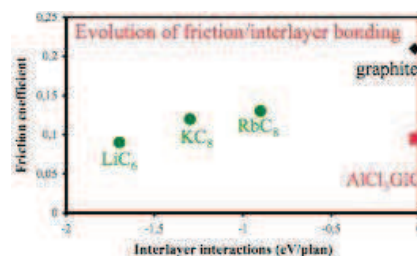


Figure 2: Friction coefficient as a function of the calculated interlayer interaction intensities.

As expected electrophilic intercalated GICs, which present low intrinsic friction, also present low interlayers interactions (lower than graphite) according to the classical interpretation of tribologic properties of lamellar compounds. The very high interlayer interactions in the case of the nucleophilic GICs associated also with friction coefficient lower than graphite is surprising. It demonstrates that friction properties are not simply related to interlayer interactions but also to other parameters such as the mobility, in the van der Waals gap, of the intercalated species. This last hypothesis is strongly suggested by the friction coefficient increase recorded from Li to Rb ions.

## 4. References

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