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

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1. Introduction

It is classically admitted that the goodfriction 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 propertiesof Graphite Intercalated Compounds (GICs) in order to better understand thetribologiclamellar compounds. In order to modulate the interlayer interactions, two types of intercalated species were used, electrophylic species ($AlCl_3$, $FeCl_3$, $SbCl_5$) 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

Tribologic results collected on the various GICs are presented in figure1.

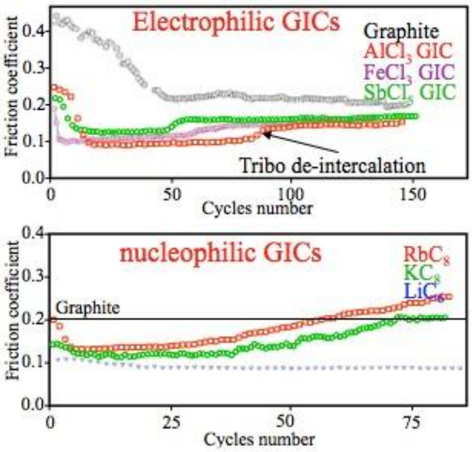

Figure 1: Evolution of friction coefficients as a function of cycles number for the two GICs families.

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 compoundspresents 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.

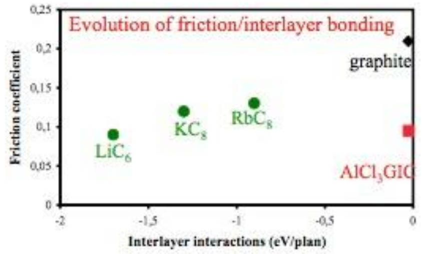

Figure 2: Friction coefficient as a function of the calculated interlayer interaction intensities.

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 nucleophilicGICs 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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