Taiho Kogyo Tribology Research Foundation

Main report

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Theme: Wear and Tribochemical Reactions in Sliding Contacts

1. Progress and result of the research

The proposed research specifically aimed to shed light on controversies relating to how boundary films initiate and understand lubricant degradation, while replying to four fundamental tribological questions; for each of these questions a thorough study was performed, assessing the underlying mechanisms by which the charge of the surfaces varies for different materials and under different sliding conditions and how this influences the interaction with the lubricant molecules.

i. How and to what extent does triboemission control surface state?

This work was a continuation of studies supported by TTRF 2011 no.11A01, which is a precursor to this project. The newly developed measurement system was used to obtain information of the charging of the surface and emission events during the sliding of a simulate asperity contact. Results from DLC coated steel specimens show how the charge of the surface is related to the emission and how this depends on the wear [1].

Sliding on the DLC coating generates emission of negative charges therefore accumulation of positive charge for the DLC surface (Figure 1a). This suggests that the surface charges positively, at least partly due to electrons leaving the surface. The failure of the coating instead causes the reduction of the emission intensity and the charge, the exposure of the metal substrate switches the contact from being diamond/DLC to being diamond/steel, preventing the accumulation of opposite charge on each of the two counter bodies. Both the wearing and the failure of the coating as proven by white light interferometry scans of the specimen (Figure 1b).

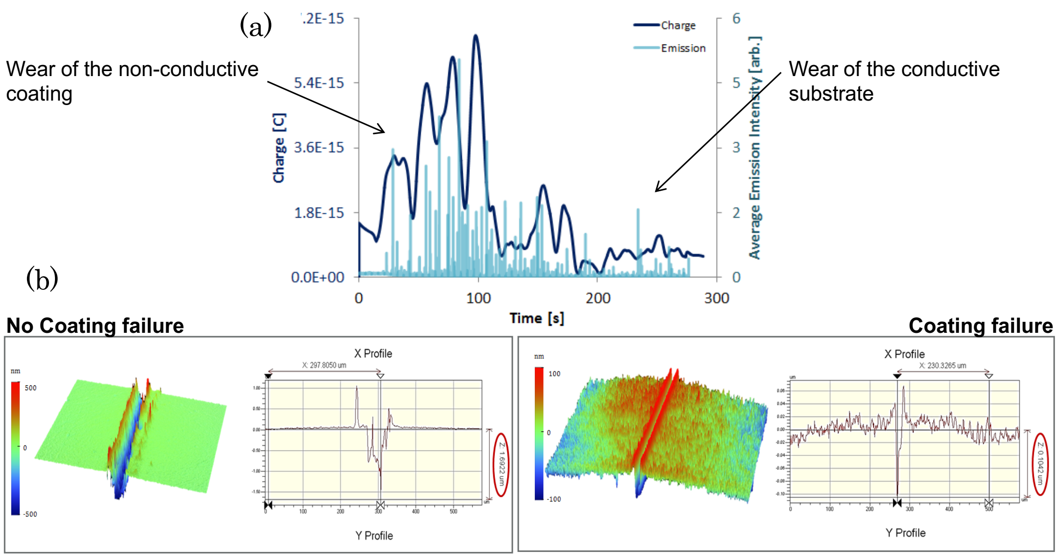

Figure 1 a) Comparison of emission and surface charge, b) WLI of the specimen surface after wear of the coating wear and coating failure

ii. Electronic surface state acquired during sliding, which will detect changes in the electrical and structural state of the surface.

The same tribometer was used to test silica specimens and same mechanisms were revealed: surface charging and emission depend on wear (Figure 2a). Furthermore, a theoretical approach provided insights into the mechanism of surface charging at atomic level (interactions between silica and diamond). The theoretical analysis conducted to unravel the charging mechanisms suggested by the experimental tests shows that at the interface between the diamond and alpha-quartz silica slab there is a transfer of charge due to the contact between the two surfaces (Figure 2b). In particular, silicon atoms lose electrons in favour of carbons atoms, leaving the silica slab positively charged as expected. Additional dynamic analysis show that disruption mechanisms generated by the sliding between the two slabs cause breaking of bonds and removal of material influencing the variation of the charge of the surfaces [2].

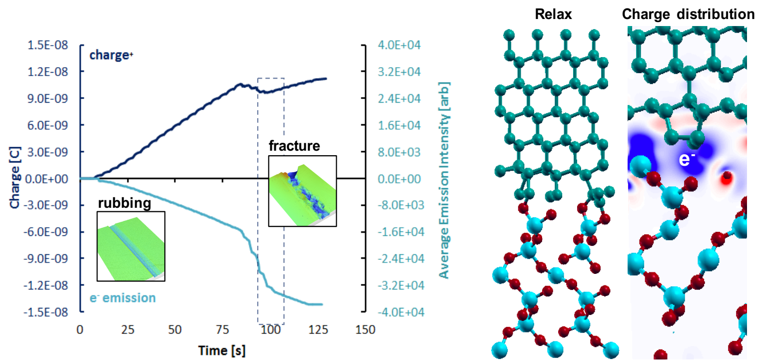

Figure 2 a) Comparison between emission and surface charge and WLI scans of the specimen, b) Charge distribution at the interface.

iii. What is the composition and structure of lubricants?

In order to explore the effect of electronic properties on tribological interactions, an *ab-initio* modelling approach was followed, starting from the study of solid lubricants. Polytetrafluoroethylene (PTFE), commercially known as Teflon, has been chosen as solid lubricant because of its unique characteristics. It is one the most effective insulating polymers for a wide range of applications, due to its peculiar electronic, mechanical and thermal properties. First-principles approach was used to elucidate its structural and electronic properties [3].

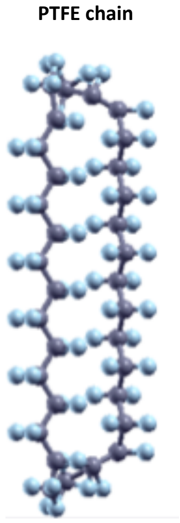

Figure 3 Atomic structure of PTFE chain.

iv. How is friction and wear behaviour related to the lubricant interaction with the surfaces in contact?

An open-source modelling tool has been created to predict the chemical processes between lubricant and surfaces. Adhesion and chemical reaction can be predicted for different materials and surfaces and compared with experimental results obtained by means of the, now, fully equipped test rig [4, 5].

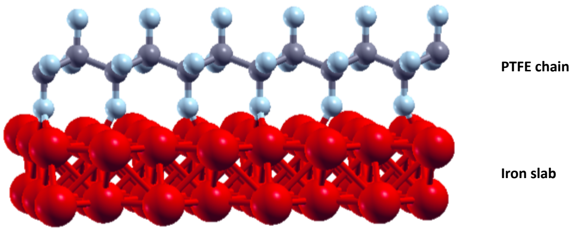

Figure 4 Surface-lubricant interaction model.

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2. Subjects remain to be solved in future/Subjects required further investigation

Research is continuing to investigate experimentally and computationally the influence of surface charge on lubricated contacts. Friction and wear will be evaluated for different materials and different contact conditions.
The tribometer and the computational model developed through the TTRF Grant will contribute significantly to this research and TTRF contribution's will also be acknowledged in the forthcoming articles.

3. Plan and past presentation or publication of your research results

These novel results, obtained partly using the resources provided through this grant, were recently published in Coatings and the Journal of Chemical Physics C. A conference proceeding from the APS March 2018 meeting has also been published. All outputs have acknowledged the Taiho Kogyo Tribology Research Foundation. Two other journal papers are currently under submission – see full list below:

[1]. "The use of triboemission imaging and charge measurements to study DLC coating failure"
A. Ciniero[1*], Julian Le Rouzic[2], T. Reddyhoff[1]
1 Imperial College London, 2 Université de Poitiers – France
Coatings (2017), 7(8), 129

[2]. "An experimental and theoretical approach to study the link between Triboemission and Tribocharging"
A. Ciniero[1*], D. Dini[1], T. Reddyhoff[1]
1 Imperial College London,
APS March Meeting 2018, (2018)

[3]. "First-Principles Insights into the Structural and Electronic Properties of PTFE in its High-Pressure Phase (Form III)"
G. Fatti[1], M.C. Righi[1], D. Dini[2], **A. Ciniero**[1,2*]
1 University of Modena, 2 Imperial College,
The Journal of Physical Chemistry C (2019) (In Press)

[4]. "An ab initio study of tribocharging during sliding"
A. Ciniero[1,2*], M.C. Righi[1], D. Dini[2]
1 University of Modena, 2 Imperial College
(to be submitted, Langmuir)

[5]. "Influence of surface charge in lubricated contacts"
A. Ciniero[1,2*], M.C. Righi[1], D. Dini[2]
1 University of Modena, 2 Imperial College
(to be submitted, Tribology International)

The recent results were presented at i) WTC 2017, Beijing, China ii) APS March Meeting 2018, LA, USA iii) STLE Frontiers – Tribology Conference 2018, Chicago, USA; and they will be presented at ITC 2019, Sendai, Japan.

Furthermore, the research conducted by Dr Ciniero resulted in the establishment of a collaboration with Dr Righi at the University of Modena and Reggio Emilia and the award of a Marie-Curie Actions grant (Award number 798245).