Wear, plasticity, and rehybridization in tetrahedral amorphous carbon

T. Kunze[1], M. Posselt[2], S. Gemming[2], G. Seifert[1], A. R. Konicek[3], R. W. Carpick[3], L. Pastewka[4], M. Moseler[4]

[1]Theoretical Chemistry, University of Technology Dresden, D-01662 Dresden, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, D-01314 Dresden, Germany
[3]Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, USA
[4]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstrasse 11, D-79108 Freiburg, Germany

Wear and friction in self-mated tetrahedral amorphous carbon (ta-C) films is studied by molecular dynamics and compared to results of near-edge X-ray absorption fine structure spectroscopy. The simulations demonstrate the formation of a soft amorphous carbon (a-C) transfer layer with increased sp^2 content, which grows faster than the a-C tribolayer found on self-mated diamond sliding under similar conditions. The faster $sp^3 \rightarrow sp^2$ transition in ta-C is explained by easy breaking of prestressed bonds in a finite, nanoscale ta-C region, whereas diamond amorphization occurs at an atomically sharp interface. A detailed analysis of the underlying rehybridization mechanism reveals that the $sp^3 \rightarrow sp^2$ transition is triggered by plasticity in the adjacent a-C. Rehybridization therefore occurs in a region that has not yet experienced plastic yield. A detailed characterization of the a-C transfer layer reveals the absence of well-ordered graphitic structures. The resulting soft a-C tribolayer is interpreted as a precursor to the experimentally observed wear.

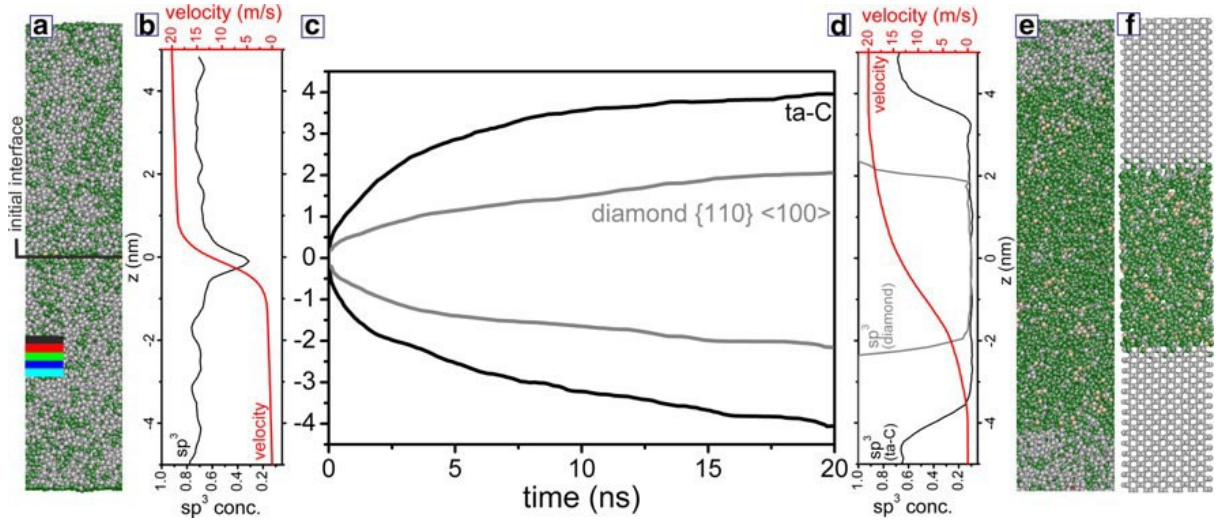

Figure 1: (a) side-view snapshot of the ta-C/ta-C tribosystem after 0.1 ns of sliding. Atoms are color- coded according to their atomic coordination: white – sp^3, green- sp^2, yellow – sp^1, (b) sp^3 concentration (black curve) and velocity profile (red curve) across the ta-C/ta-C tribocouple, (c) evolution of the upper and lower boundary of the a-C tribofilm formed between two ta-C surfaces (black curve) compared to a corresponding film formed between two diamond {110} surfaces rubbed in <100> direction (gray curve), (d) sp^3 concentration (black curve for ta-C and gray curve for diamond) and velocity profile of the ta-C system (red curve) after 20 ns of sliding, (e) and (f) are side- view snapshots of the ta-C/ta-C and diamond/diamond tribosystems after 20 ns sliding.

T. Kunze *et al.*, Tribol. Lett. **53**, 119 (2014).

Quantifying touch-feel perception: Tribological Aspects on a new artificial finger design

Hui Niu[1], Xianping Liu[1], Hin Kwan Wong[2]

[1]School of Engineering, University of Warwick, Coventry CV4 7AL, UK
[2]Warwick Manufacturing Group, University of Warwick, Coventry CV4 7AL, UK

The human skin tribology is a research topic that has continuously attracted scientific studies over the past years. It has applications in enabling the sense of touch in robotics and enhancing touch-feel ergonomics in products [1].Artificial fingers are able to characterise surface roughness by emulating the ability of human fingertip to sense friction.

To mimic human finger doing so by stroking on the object this, an artificial finger is combined with a linear flexure mechanism and a reciprocal stage to form a friction measurement device. By measuring the contact force and friction force simultaneously, the friction coefficient can be calculated and therefore the surface roughness characterised. This paper continues on earlier work [2] on the friction measurement device and presents a new design capable of measurement profiles closely matching that obtained from a human finger. In the original setup in [2], the friction coefficient was measured manually by applying pressure on the test material with a finger.

However, this friction measurement rig was extremely sensitive to the humidity of the human fingertip and may become inconsistent if the test were not performed in one sitting. The original design was later improved by addition of a roller-on-block structure in order to replace the human finger and therefore reduce the variance of the applied contact force [2]. The rollers were made of steel, brass and silicone rubber materials whose Young's moduli were close to that of a human fingertip.

The current artificial fingertip design used in this paper (Fig. 1) has a multi-layered construction comprising of the cover layer and the filler layer, both made of silicone rubber with different hardness, and an internal bone support structure made of aluminium. Instead of having a roller mechanism, the artificial finger is fixed on a linear stage that enables a reciprocating back-and-forth motion more representative of human touch movement. Experimentation was carried out to measure surface frictions of aluminium and steel plates with different roughness, under different contact forces and different stroking speeds. High correlations (R=0.85~0.98) between artificial finger friction measurements and those obtained by human finger were observed for the steel samples and the milled aluminium samples. The results show that the artificial finger can be very close to the human finger in terms of the friction sensing characteristics. The results also indicate that in the low roughness range, the friction coefficient decreases as the contact force increase, but the difference is slight in the high roughness range. Finally, the measured friction coefficient increases with the linear stage sliding speed.

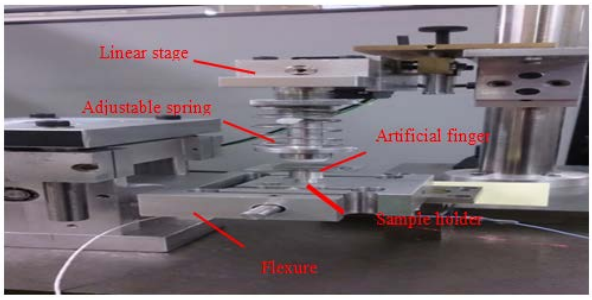

Fig.1 The artificial finger set up with the linear stage

[1] Childs T H C and Benson B 2007 Human tactile perception of screen-painted surfaces: self-report and contact mechanics experiments Proc. Inst. Mech. Eng. J: 221 427–41
[2] Xian Ping Liu, Zhaoyang Yue, Zhijian Cai, Derek Chetwynd and Stuart T Smith. Quantifying touch-feel perception: tribological aspects. Meas. Sci. Technol. 19 (2008), doi:10.1088/0957-0233/19/8/084007.

Multiscale estimating technique of rubber friction on surface asperities depending on sliding velocity

Hiro Tanaka[1], Kimiyasu Yoshimura[1], Junpei Aramaki[1], Satoshi Izumi[1], Shinsuke Sakai[1], Hiroshi Kadowaki[2]

[1]University of Tokyo, 7-3-1, Hongo, Bunkyo-Ku, Tokyo, Japan
[2]Bridgeston Corporation, 3-1-1, Ogawahigashi-Cho, Kodaira-Shi, Tokyo, Japan

According to Persson's statement [1][2], the friction coefficient of a rubber is mainly determined by both the rubber's viscoelasticity and the surface property on multiscale asperities which can be represented by surface roughness power spectrum (SRPS). In this study, we conduct friction testing for a carbon filled rubber sliding on dry surface asperities. Based on the experiment results, we estimate the net friction coefficient related to energy dissipation resulting from cyclic deformations of the rubber, which derived from the Persson's mathematical model.

The friction coefficient developed by Persson [1] reads

$$\mu_{\mathrm{Persson}} = \frac{1}{4\pi}(q_0 h_0)^2 H \int_1^{q_1/q_0} \mathrm{d}\zeta \zeta^{-2H+1} P(\zeta) \int_0^{2\pi} \mathrm{d}\phi \cos\phi \,\mathrm{Im}\frac{E(\zeta q_0 v \cos\phi)}{(1-\nu^2)\sigma_0} \qquad (1)$$

In our procedure, the Hurst exponent H and roll-off wavelength $q0$ were obtained by the measured SRPS (see Fig. 1), and the complex elastic modulus E was represented by the generalized Maxwell model identified by the viscoelasticity measurement of a rubber specimen. In Eq. (1), the cut-off wavelength q_1 is known as a free parameter. Hence we determined q_1 so that the velocity dependency of μ_{Persson} agreed well with that of μ_{exp} measured by the friction test. Figure 2 shows the μ-v curves: the solid line indicates the experiment value and the dashed line does the value of μ_{Persson} estimated from the relationship of $\mu_{\mathrm{Persson}} \approx \mu_{\mathrm{exp}} - \mu_{\mathrm{offset}}$, assumed that μ_{offset} doesn't depend on sliding velocity.

The part of this work was supported by the Japan Society for the Promotion of Science under the grand-in-aid for scientific research (B) (JSPS KAKENHI Grand No. 24360044).

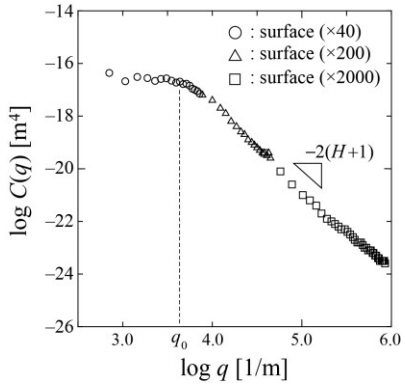

Figure 1: Surface roughness power spectrum measured by a laser microscope.

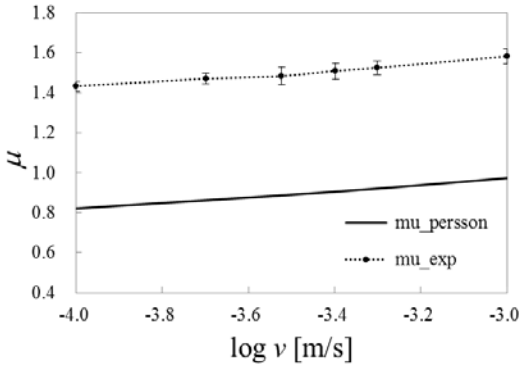

Figure 2: □-v curves: the experiment value and the net value estimated using Eq. (1).

[1] B.N.J. Persson, J. Chem. Phys. **115**, (2001), pp. 3840–3861.
[2] B.N.J. Persson et al., J. Phys.: Condens. Matter. **17**, (2005), R1–R62.

Nanoindentation and wear of graphene-covered surfaces

Andreas Klemenz[1], Lars Pastewka[1], Michael Moseler[1,2]

[1]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany
[2]University of Freiburg, Physics Department, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Graphene has the highest stiffness and the highest breaking strength that have ever been measured in an experiment [1]. If these properties could be transferred to the surface of a soft material, graphene could be used as the thinnest possible protective coating. Usage of graphene for this purpose requires a deep understanding of its influence on wear and tribological processes. Since all relevant processes take place on an atomic length scale, atomic force microscopy is usually used for experimental investigations. Such studies can give basic insight into the system behavior, but detailed analyses are often difficult. Details of the setup like the surface roughness of the indenter cannot be controlled but can have a strong influence on experimental results. Roughness has a considerable influence on the stress distribution under the tip [2] and can modify the result of a work of adhesion measurement by more than an order of magnitude [3]. Apart from this, it is often not possible to perform an indentation and simultaneously observe the surface. In the special case of a graphene-covered surface, it is therefore difficult to tell, if the graphene has ruptured at a certain point and which signature in a force penetration curve indicates graphene rupture.

In atomistic simulations, the setups can be controlled exactly and every interesting property of the material can be monitored simultaneously. In this work, we therefore use quasistatic simulations of indentation processes. We use platinum as a model for soft surfaces and investigate the behavior of Pt (111) surfaces coated with single layers of graphene when indented with rigid tips. Since the relevant processes can be rather slow, we use a quasistatic approach as a model for infinitely slow indentations. We vary the size and shape of the indenter and discuss the influence of graphene coatings on the hardness of the surface. Finally we compare our results with those of an experimental study.

[1] C. Lee et al. Science 321, 385 (2008)
[2] B. Luan, M.O. Robins, Nature 435, 929 (2005)
[3] T.B.D. Jacobs et al. Tribol. Lett. 50, 81 (2013)

Seamless elastic boundaries for atomistic calculations

Lars Pastewka[1], Tristan A. Sharp[2], Mark O. Robbins[2]

[1]Fraunhofer IWM, [2]Johns Hopkins University

The elastic response of an infinite bulk crystalline solid with a free surface can be renormalized into a linear operator, the surface Green's function that acts on the surface's degrees of freedom only [1]. We here present general transfer matrix and renormalization group formulations that allow the computation of the elastic surface Green's function from the knowledge of the interatomic interaction [2]. Our approach naturally allows a treatment of multi-atom unit cells that are necessary to couple a renormalized substrate to a full atomistic system that interacts via long-ranged forces. The substrate interaction is treated exactly up to harmonic order and the full system comprising atomistic and elastic boundary regions is described by a single Hamiltonian. This concurrent multi-scale coupling enables simple, seamless semi-infinite elastic boundary conditions for atomistic simulations where near-surface deformations occur, such as nanoindentation, contact, friction, or fracture. We demonstrate this method on problems from contact mechanics and tribology.

[1] C. Campañá, M.H. Müser, Phys. Rev. B 74, 075420 (2006)
[2] L. Pastewka, T.A. Sharp, M.O. Robbins, Phys. Rev. B 86, 075459 (2012)

Improving Estimates of Fretting Wear Rates through Microscale Simulations

Areg V. Hayrapetian[1], Michael J. Demkowicz[2]

[1]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
[2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Fretting wear is a problem that comes up in many engineering applications. Work-rate models, such as Archard's law [1], with constant empirical wear coefficients are commonly used to estimate wear rates for most wear applications. Their shortcoming is that they cannot describe wear under conditions that may change the wear coefficient. To improve on the work-rate model, a model of fretting wear is needed that can simulate wear mechanisms at the micron length scale. This goal necessitates simulation methods capable of modeling elasticity, fracture, contact, generation of wear debris, and tracking and contact interaction of the third-body wear debris particles.

We present work in progress on a new modeling framework with these capabilities. This modeling framework allows for simulations of the fretting wear mechanics at the micron length-scale such as the fracture of asperities on two sliding brittle surfaces. A snapshot of a preliminary simulation of this type completed on a small-sized system can be seen in Figure 1. Similar simulations on larger systems will allow us to better understand the behavior of fretting wear as a function of parameters such as the normal contact load, slip amplitude of the oscillatory sliding, surface roughness, and type of fretting motion. The results of these simulations will be used to construct a wear mechanism map for fretting wear that predicts variations of wear coefficients with the prior stated parameters in order to eventually better estimate wear rates under a variety of operating conditions.

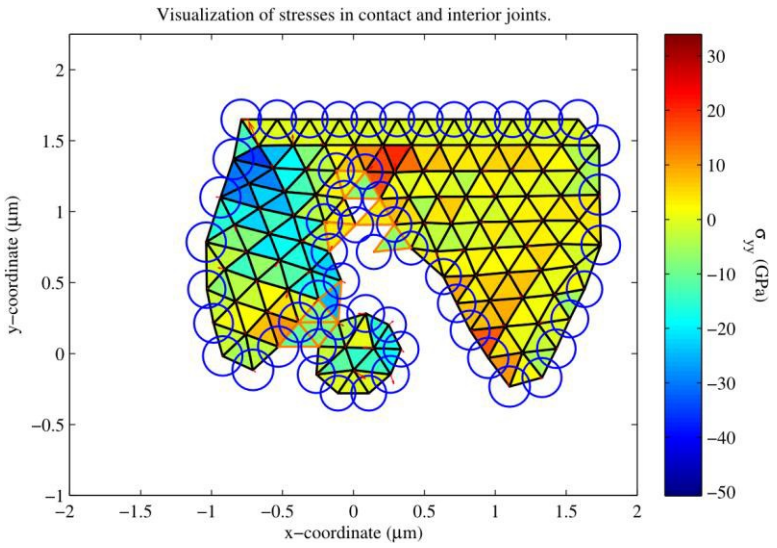

Figure 1: Snapshot of asperity fracture simulation.

This project was supported by the Consortium for Advanced Simulation of Light Water Reactors (CASL): a Department of Energy (DOE) Energy Innovation Hub.

[1] J. F. Archard. J. of Appl. Phys. **24**, 981 (1953).

Theoretical modeling and molecular dynamics simulation of atomic scale wear: A combined study

Yuchong Shao, Michael L Falk

Johns Hopkins University

Frictional running-in and material transfer in wear take place at the micro- and nano-scale but the fundamental physics remains unclear. In recent years, various mechanisms including cluster-detachment process and atom-by-atom attrition have been reported in simulation and experimental work.

Here we propose a multi-bond dynamics model based on Filippov et al [Phys. Rev. Lett. 92, 135503 (2003)] that qualitatively captures those two distinct behaviors under a unified theoretical framework. In the model, the interfacial bond formation, rupture and wear are depicted as three competing thermally activated processes. We demonstrate that depending upon the external normal stress and sliding rate, different regimes of wear behavior exhibited in such a model.

To test this theory we perform molecular dynamics simulation of a silicon-based AFM and quantified the rate of material transfer as a function of the coverage of non-bridging oxygen atoms, which has a pronounced change of the system's tribological and wear behaviors. Results show that adhesive wear takes place across the interface in an atom-by-atom fashion which remodels the tip. Comparisons to experimental data and other wear simulations are also discussed.

Multiscale Modelling for Atomic Force Microscopy

Yasuhiro Senda[1], Shuji Shimamura[1], Janne Blomqvist[2], Risto Nieminen[2]

[1]Department of Applied Science, Yamaguchi University, Yamaguchi, 755-8611, Japan
[2]COMP Centre of Excellence, Department of Applied Physics,
Aalto University, P.O. Box 11100, 00076 Aalto, Finland

Atomic Force Microscopy (AFM) is promising tool capable to providing atomic resolution images for a variety of materials. The macroscale cantilever of the AFM is oscillated in macroscale time on the surface and its resonance frequency is changed by the atomic interaction between the tip of the cantilever and the surface. The multiscale behavior of the macroscopic motion of the cantilever and the atomic interaction between the tip and the surface provides the atomic resolution image of the AFM experiment. In addition to the change of resonance frequency, the oscillation of the cantilever is damped and this energy dissipation also offers a structural atomic image. The origin of the energy dissipation, however, has been the subject of debate over the past decade.

We propose a multiscale model of the AFM using a coupling method of molecular dynamics (MD) and continuum in order to investigate mechanism of the observed energy dissipation of the AFM experiment. The motion of cantilever is described by a spring, and the atomic interaction between the tip attached on cantilever and surface is calculated by MD method as shown in the below Figure. The motions of the spring and atoms are concurrently coupled by the MD/continuum hybrid method [1,2]. The Lennard Jones potential is used as the inter-atomic interaction.

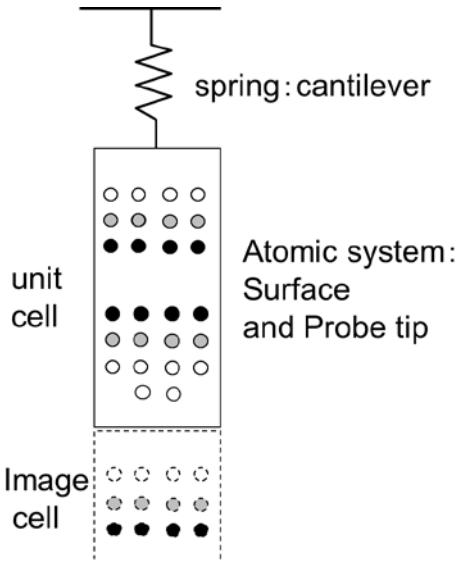

Figure: Schematic view of the multiscale model for AFM. Lennard Jones atoms are drawn by circles. Atoms drawn by solid circles are fixed.

The energy dissipation of the spring (cantilever) is calculated using the above multiscale model, and the calculated dissipation on each atomic site of the surface for Lennard Jones crystal can provide the atomic image of the surface. The mechanism of the energy dissipation in the present AFM model will be explained and discussed.

References

[1] G. Kim and Y. Senda: J. of Physics.: Condens. Matter 19 246203 (2007)
[2] Y. Senda et al, J. of Chem. Phys., 137, 154115 (2012)

Density Functional Study of Gold-Coated Iron Nanoparticles (Potential for Medical Applications)

Eyachew Misganew

Debre Tabor University, Ethiopia

In this paper, the first principle studies on the ground state structure, binding energy, and magnetic moment of gold-coated Fe_n, bare Fe_n, and their oxides, Fe_nO_2 have been carried out within a density functional formalism. The first systematic theoretical study of gold-coated iron nanoclusters, aiming at understanding the magnetic properties of this core-shell structure used in biomedical applications. The calculations based on density-functional theory focus on the effect of gold coating on the magnetic and structural properties of iron clusters of various sizes, and the reaction of the bare iron clusters with oxygen. My results show that the magnetic moment of iron nanocore with gold coating is still significantly higher than that in bulk Fe; the coupling between Fe atoms remained ferromagnetic. The improved chemical stability by gold coating prevents the iron core from oxidation as well as the coalescence and formation of thromboses in the body. Thus, it is shown that gold coating is very promising for the magnetic particles to be functionalized for targeted drug delivery. The ground states of Fe_n clusters have a magnetic moment of around 2.94 μB per atom. The O_2 molecule is found to be dissociatively absorbed and its most significant effect on spin occurs in Fe, Fe_2, Fe_5 and Fe_6, where FeO_2, Fe_2O_2, Fe_5O_2, and Fe_6O_2 show antiferromagnetic spin arrangements, respectively.

Computational Chemistry Study on Resin/Metal Interface: Tribochemical Reaction and Its Effect on Friction

Tasuku Onodera[1], Kenji Kawasaki[1], Takayuki Nakakawaji[1], Yuji Higuchi[2], Nobuki Ozawa[2], Kazue Kurihara[3], Momoji Kubo[2]

[1]Hitachi, Ltd., Hitachi Research Laboratory, 7-1-1 Omika-cho, Hitachi 319-1292, Japan
[2]Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, 6-6-11 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan
[3]WPI-Advanced Institute for Materials Research & Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

Polytetrafluoroethylene (PTFE) is a useful bearing material because it shows a low friction when rubbed against metallic surfaces. However, the tribological performance of PTFE is strongly influenced by its working environments such as humidity; wear amount is increased under low humid condition. Therefore, it is necessary to develop a novel PTFE composite material for use as bearing under dry condition. For this purpose, the mechanism of chemical interaction on PTFE/metal interface should be worked out. In this study, a computer chemistry approach was adopted for revealing the chemical phenomena at PTFE/metal interface. A tight-binding quantum chemical molecular dynamics method was used to observe the tribochemical reaction between PTFE and metallic surface. The model is shown in Figure 1(a) and is consisted of crystalline PTFE and aluminum oxide terminated partially by some hydroxyl (OH) groups. Figure 1(b) shows the final structures of this system, and a bond dissociation reaction between carbon and fluorine atoms was observed. Moreover, the bond formation reaction was found in which the dissociated fluorine atom bonded to a bare aluminum atom. The results indicate that PTFE tribochemically reacts with a aluminum surface to form aluminum fluoride as a product. The subsequent chemical reaction with environmental gaseous molecule and the effect of the unveiled reactions to the tribological property will be presented in our presentation.

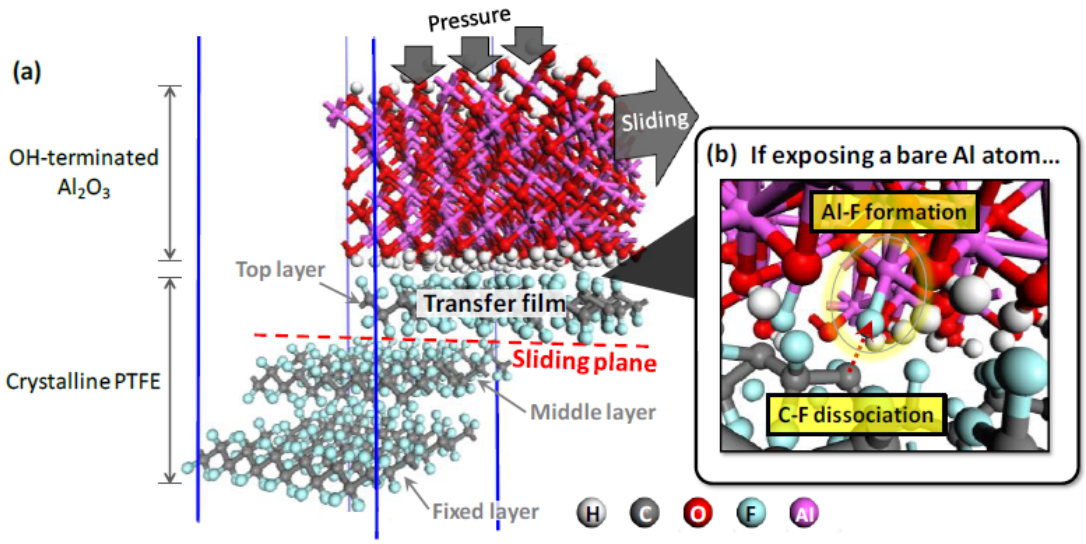

Figure 1: (a) Model structure during friction process, and (b) the tribochemical reaction.

Piston pin lubrication

Hannes Allmaier[1]

[1]Virtual Vehicle Research Center, Graz, Austria

Of all moving parts in the internal combustion engine (ICE) that can be investigated in terms of friction and lubrication, the piston pin represents a unique challenge [1]. Due to its floating movement, extreme temperatures and oil mist lubrication, this part works not only under extreme operating conditions, but is also very difficult to describe numerically. Being not fixed on any end, the piston pin is free to move, only driven by the lubricant film, which, however, is also unknown at the beginning.

A simulation method is developed that considers the thermal deformation of the piston and the piston pin and incorporates an extensive rheological model for the lubricant [2]. With this model it is possible to describe the lubricant film and with it the friction and movement of piston pin accurately as direct comparisons to experimental data show. In the following it can be used to develop measures to ensure a better lubrication of this critical part.

[1] H. Allmaier, C. Priestner, D.E. Sander, F.M. Reich, book chapter '*Friction in automotive engines*' in book '*Tribology in engineering*', Intech (2013), ISBN 980-953-307-460-8

[2] H. Allmaier, C. Priestner, F.M. Reich, H.H. Priebsch, C. Forstner, F. Novotny-Farkas, Tribology International 48, p. 93-101 (2012).

Roughness induced hysteretic behavior of adhesive contacts

Giuseppina Recchia[1], Elena Pierro[2], Giuseppe Carbone[1]

[1]Dipartimento di Ingegneria Meccanica e Gestionale, Politecnico di Bari, v.le Japigia 182, 70126 Bari - Italy
[2]Scuola di Ingegneria (SI - UniBas), Università degli Studi della Basilicata, Campus di Macchia Romana - Via dell'Ateneo Lucano 10, 85100 Potenza – Italy

In this paper we investigate the adhesive contact between a rubber block and rigid randomly rough profiles (Figure 1), in loading and unloading conditions. The roughness is assumed to be described by a self-affine fractal on a limited range of wave-vectors.

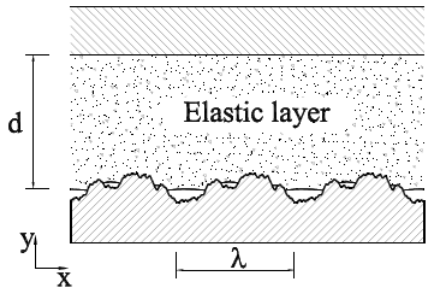

Figure 1: An elastic layer of thickness d in adhesive contact with a rough rigid substrate.

We employ a spectral method to generate such randomly rough surfaces with different root mean square roughness values and fractal dimensions. Calculations are performed for each profiles by means of an ad hoc numerical code previously developed by the authors [1-2]. The calculated data are then statistically averaged, and the contact area, the applied load are shown as a function of the penetration, both for loading and un-loading conditions. It is found that the combination of adhesion forces and roughness leads to a hysteresis loading-unloading loop, which might be unexpected for perfectly elastic materials. This result is very interesting as it shows that energy can be lost simply as a consequence of roughness vand der Waals forces. Our calculations enable us to numerically quantify such an energy loss and, in particular, to assess the influence of the fractal dimension Df and of the Duprè energy of adhesion this hysteresis process.

[1] G. Carbone, M. Scaraggi, U. Tartaglino, Eur Phys J E Soft Matter, **30** (1), 65-74 (2009).
[2] G. Carbone, L. Mangialardi, J Mech Phys Solids, **56** (2), 684-706 (2008).
[3] J.A. Greenwood, J. B. P. Williamson, Proc R Soc Lond A Math Phys Sci, **295**, pp. 300-319.
[4] B.N.J. Persson, J Chem Phys, **115**, 3840 (2001).
[5] A.W. Bush, R.D. Gibson, T.R. Thomas, Wear , **35**, 87 (1975).
[6] T.R. Thomas, (Chapter 8), Longman Group Limited, New York (1982). [7] J.A. Greenwood, Wear, **261**, 191-200 (2006).
[8] J.A. Greenwood, J Tribol, **107**, 501-504, (1985).
[9] G. Carbone, F. Bottiglione, Meccanica, DOI: 10.1007/s11012-010-9315-y, (2010).
[10] G. Carbone, J Mech Phys Solids, **57** (7), 1093–1102 (2009).
[11] G. Carbone, F. Bottiglione, J Mech Phys Solids, **56** (8), 2555-2572 (2008).
[12] G. Carbone, E. Pierro, J Adhes Sci Technol, 2555-2570, 2012.

Molecular dynamics study of automotive lubricants: linking molecular structure and friction

Michael Doig[1], Philip J. Camp[1], Chris P. Warrens[2]

[1]School of Chemistry, Joseph Black Building, University of Edinburgh, West Mains Rd, Edinburgh, EH9 3JJ, UK
[2]BP Technology Centre, Pangbourne, RG8 7QR, UK

Lubricant oils are used to reduce friction and wear in a wide range of industrial and mechanical processes. Lubricant additives play a vital role in the oils' overall performance, particularly surface-active additives which can significantly affect the tribological properties of solid surfaces. However, there is insufficient understanding of the link between the atomic-level structure of tribofilms and the macroscopic properties such as friction, to direct the development of new lubricant formulations.

Using large-scale molecular dynamics simulations, we investigate a range of lubricated systems, studying the structural properties of surface-adsorbed tribofilms on metal-oxide surfaces, and how they vary with temperature, pressure, surface coverage and shear rate. Several important trends are identified linking molecular isomerism and architecture with the structure and stability of the adsorbed films. In addition, the simulation results are used to gain insight on recent experimental measurements of film structure [1]. Some examples of the systems studied include oleic acid and stearic acid films lubricated by squalane (see figure 1) [2], and hexadecylamine films lubricated by dodecane [3], both adsorbed on iron oxide surfaces.

The friction coefficients in these systems are computed and analysed with reference to the structure of the adsorbed films, to yield new insights on the intimate link between the molecular properties of lubricants and the macroscopic frictional properties of lubricated systems.

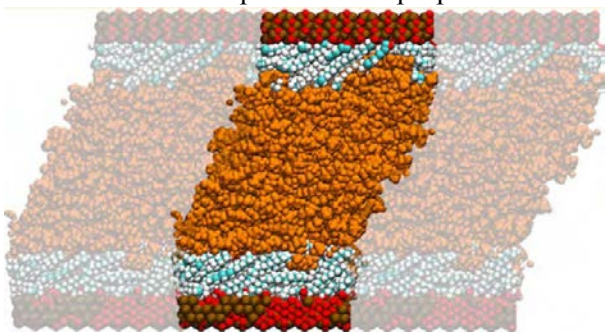

Figure 1: Lubricated system of oleic acid adsorbed on iron oxide lubricated by squalane base oil, under applied shear.

This work was supported through a CASE studentship by BP International Ltd and EPSRC(UK.

[1] M. Wood, R. J. L. Welbourn, T. Charlton, A. Zarbakhsh, M. T. Casford and S. M. Clarke *Langmuir*, **29**, 13735–13742 (2013)
[2] M. Doig, C. P. Warrens, and P. J. Camp *Langmuir* **30**, 186-195 (2014) [3] M. Doig and P.J. Camp In preparation.