

# Café Scientifique invité

Amphi 203 ECL

Vendredi 28 juin 2013 - 13h-15h

## Wear in diamond and hydrogen-free diamond-like carbon

Prof. M. MOSELER

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In the first part of this talk wear in tetrahedral amorphous carbon (ta-C) and diamond is studied by molecular dynamics using a bond-order potential that has been modified to reproduce the tribological behaviour of carbon materials [1]. We observe the formation of a soft, mainly sp<sup>2</sup> hybridized amorphous carbon (a-C) tribolayer which grows faster for ta-C than for diamond surfaces sliding under otherwise similar conditions [2]. The faster sp<sup>3</sup> to sp<sup>2</sup> transition in ta-C is explained by easy breaking of prestressed bonds in a nanoscale ta-C region triggered by plasticity in the adjacent a-C while the diamond/a-C transition occurs at an atomically sharp interface [3]. In the second part of my talk, experimental and theoretical insights into the wear and running-in of W/WC tribo-couples will be presented [4].

- [1] L.Pastewka, M.Mrovec, M.Moseler, P.Gumbsch, Bond order potentials for fracture, wear and plasticity, *MRS Bulletin* 37, 493 (2012)  
 [2] Tim Kunze, Matthias Posselt, Sibylle Gemming, Gotthard Seifert, Andrew R. Konicek, Robert W. Carpick, Lars Pastewka and Michael Moseler, *Wear, plasticity, and rehybridization in tetrahedral amorphous carbon*, Submitted. (2013)  
 [3] Lars Pastewka, Stefan Moser, Peter Gumbsch, Michael Moseler, , *Anisotropic mechanical amorphisation drives wear in diamond* *Nature Materials* 10, 34 (2011)  
 [4] P.Stoyanov, P.Romero, T.T. Järvi, L.Pastewka, M.Scherge, P.Stemmer, A.Fischer, M.Dienwiebel, M.Moseler, *Experimental and atomistic investigation of the third body formation process in dry tungsten/tungsten-carbide tribo couples*. *Tribology Letters* (2013)

## Friction, Adhesion, and Wear Behavior of Ultrananocrystalline Diamond

Prof. Robert W. CARPICK

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A lack of understanding of nanoscale friction and wear is a primary limitation for small-scale devices such as atomic force microscopy (AFM) probes and micro- or nano-electronic mechanical systems, and is also relevant for understanding friction and wear in larger-scale contacts. Ultrastrong carbon-based materials have exceptional friction and wear characteristics, but only under certain conditions. I will describe measurements aimed at uncovering fundamental insights into friction and wear for these materials, and physical origins to the observed variation in their properties.

I will first present studies of macroscopic friction and wear in ultrananocrystalline diamond (UNCD) thin films, where we observe that tribochemical effects are critical. In particular, friction and wear are governed by a competition between the dissociative adsorption of water vapor with bond breaking and reforming at the sliding interface. This results in a remarkably sharp, reversible transition between low and high friction as the partial pressure of water is varied<sup>1-3</sup>.

I will then discuss the role of roughness in determining nanoscale adhesion. It is well known that surface roughness affects adhesion at macro- and microscopic scales, but atomic-scale roughness of asperities, including sharp tips used for advanced AFM, is rarely measured or accounted for. We characterized the atomic-scale roughness of UNCD and diamondlike carbon (DLC) AFM probes, and measured the corresponding effect on adhesion using experimental techniques. Adhesion tests were conducted inside of a transmission electron microscope (TEM). This in situ methodology allowed the surface roughness to be characterized with sub-nanometer resolution immediately before and after contact. Experimental results were compared with complementary simulations conducted using molecular dynamics (MD). The range of roughness considered spanned from 0.03 to 1.58 nm. Over this range, the work of adhesion decreased by more than an order of magnitude as roughness increased, with a consistent trend observed between experiments and simulations. The trend was accurately described by a simple analytical model. These results demonstrate the high sensitivity of adhesion to interfacial roughness down to the atomic limit<sup>4</sup>.

1.Konicek, A.R., Grierson, D.S., Gilbert, P.U.P.A., Sawyer, W.G., Sumant, A.V. and Carpick, R.W. Origin of Ultralow Friction and Wear in Ultrananocrystalline Diamond. *Phys. Rev. Lett.* 100, 235502/1-4 (2008).

2.Hamilton, M.A., Konicek, A.R., Grierson, D.S., Sumant, A.V., Auciello, O., Sawyer, W.G. and Carpick, R.W. Environmental Performance Limits of Ultrananocrystalline Diamond Films. 2008 Proceedings of the STLE/ASME International Joint Tribology Conference, IJTC 2008, 9-10 (2009)

3.Konicek, A.R., Grierson, D.S., Sumant, A.V., Friedmann, T.A., Sullivan, J.P., Gilbert, P., Sawyer, W.G. and Carpick, R.W. Influence of Surface Passivation on the Friction and Wear Behavior of Ultrananocrystalline Diamond and Tetrahedral Amorphous Carbon Thin Films. *Phys. Rev. B* 85 (2012).

4.Jacobs, T.D.B., Ryan, K.E., Keating, P.L., Grierson, D.S., Lefever, J.A., Turner, K.T., Harrison, J.A. and Carpick, R.W. The Effect of Atomic-Scale Roughness on the Adhesion of Nanoscale Asperities: A Combined Simulation and Experimental Investigation. *Tribol. Lett.* 50, 81-93 (2013)