Towards an atomic scale understanding of wear in carbon materials and metals

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Despite the fact that diamond and diamond-like carbon (DLC) [1] coatings are used in an increasing number of applications, not much is known about the atomic scale processes that cause the wear of these films. For instance, the microscopic mechanisms that occur in DLC films in tribological applications [2,3] or the polishing of diamonds are still poorly understood [4]. Molecular dynamics is ideally suited to gain a deeper understanding of the underlying wear processes. In this talk a variety of atomistic simulations employing a novel Brenner bond order potential [5,6] that has been corrected for a faithful description of bond breaking processes are reported.

For diamond polishing, the occurrence of soft polishing direction can be related to the generation of thick amorphous soft layers [7] that are not stable with respect to mechanical plowing or oxidative etching by ambient air [8]. The velocity of the diamond/amorphous-carbon interface depends crucially on the diamond surface orientation with the highest speed found for (110) surfaces that are rubbed in the (001) direction, while the lowest interface speed was observed for the diamond (111) surface. These finding are in perfect agreement with a 600 years old experimental knowledge of diamond polishers. The anisotropy of the wear is rationalized within a rate model based on a yield criterion for single bonds at the crystalline/amorphous interface [7]. Wear in hydrogen-free DLC films follows a similar route. The initial mainly 4-fold coordinated carbon network exhibits a mechanically driven phase transformation into a weak sp^2 phase that can be easily removed from the sliding interfaces [9].

The talk concludes with our first insights into the atomic scale wear mechanism in metallic tribosystem by reporting on wear particle generation in nanocrystalline coinage metal films.

[1] M. Moseler, P. Gumbsch, C. Casiraghi, A. Ferrari, J. Robertson, The ultrasmoothness of diamond-like carbon surfaces, **Science** 309, 1545 (2005)
[2] L.Pastewka, S. Moser, M. Moseler, B. Blug, S. Meier, T. Hollstein, P. Gumbsch, The running-in of amorphous hydrocarbon tribocoatings: a comparison between experiment and molecular dynamics simulations, **Int. J. Mat. Res.**, 10, 1136 (2008)
[3] L.Pastewka, S.Moser, M.Moseler, Atomistic insights into the running-in, lubrication, and failure of hydrogenated diamond-like carbon coatings, **Tribo. Lett.** 39, 49 (2010)
[4] J.Hird and J.Fields, Diamond polishing, **Proc. R. Soc. Lond.** 460, 3547 (2004)
[5] L.Pastewka, M.Mrovec, M.Moseler, P.Gumbsch, Bond order potentials for fracture, wear and plasticity, **MRS Bulletin** 37, 493 (2012)
[6] L. Pastewka, P. Pou, R. Perez, P. Gumbsch, M. Moseler, Describing bond-breaking processes by reactive potentials: the importance of an environment-dependent interaction range, **Phys. Rev. B** (R) 78, 161402 (2008)
[7] Lars Pastewka, Stefan Moser, Peter Gumbsch, Michael Moseler, , Anisotropic mechanical amorphisation drives wear in diamond **Nature Materials** 10, 34 (2011)
[8] Gianpietro Moras, Lars Pastewka, Johan Schnagl, Peter Gumbsch, Michael Moseler, Progressive shortening of carbynoid structures through O_2-induced cleavage, **J. Phys. Chem. A** 115, 24653 (2011)
[9] 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)