Towards an atomistic understanding of wear in diamond and diamond-like carbon

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Despite the fact that diamond and diamond-like carbon coatings (DLC) [1] 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 lecture a variety of atomistic simulations employing a novel Brenner bond order potential [5] 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 layers that are not stable with respect to oxidation. 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 [6].

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. The lecture concludes with first atomistic insights into the wear of metallic nano granular films.


