

Surface roughness evolution in atomistic simulations of adhesive wear: from asperity collision to three-body configuration

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Surface roughness is relevant to all the phenomena and processes that take place at the interface between two bodies, like adhesion, contact, friction, and wear. Understanding the relation between surface roughness evolution and wear is therefore key in several fields: from the optimization of the design of manufactured objects to the understanding of fault slip during earthquakes. Experimental evidence and field observation show that worn surfaces are self-affine^{1,2}. The complexity of the wear phenomenon makes the understanding of the underlying physics a challenge though, and complicates the quest for simplified, yet sufficiently accurate models capable of describing the wear process. The same reason does not make numerical modeling simple either, as continuum approaches cannot capture the aforementioned complexity, while discrete approaches are limited by the computational cost necessary to investigate length and time scales relevant to engineering applications.

A recently developed atomistic simulations approach³ permitted us to overcome the length-scale limitation. This allowed us to gain significant insights on the physics of surface roughness evolution during adhesive wear processes. Our results show that the evolution of the surface morphology can be split in two different phases: running-in and long-term sliding. In the first phase, two surfaces come into contact at the asperity level. We find³ that a material-dependent critical length scale governs the ductile-to-brittle transition: if the junction formed by the two colliding asperities is smaller than this critical length, the asperities deform plastically, otherwise they break. This is a fundamental turning point for the surface roughness evolution: if no junction is large enough, the surfaces will smooth continuously until they weld together. On the contrary, when the junction size is sufficiently large, a debris particle is formed by fracture, thus creating roughness.

The evolution of the surface roughness after running-in is characterized by a different configuration. In our simulations, the debris particle formed upon the initial contact is constrained to roll between the two surfaces and the system transitions to a three-body configuration. The changes in the morphology are then governed by the contact between the debris particle and the surface. Over long time-scales, this leads the worn surfaces to exhibit a self-affine morphology.

In this presentation we will also address the relation between tangential work and wear volume⁴ and the interaction between multiple asperities at the onset of wear⁵.

- [1] Persson, B., Albohr, O., Tartaglino, U., Volokitin, A. & Tosatti, E. On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion. *J. Phys.: Condens. Matter* **17**, R1 (2004).
- [2] Renard, F., Candela, T. & Bouchaud, E. Constant dimensionality of fault roughness from the scale of micro-fractures to the scale of continents. *Geophys. Res. Lett.* **40**, 83–87 (2013).
- [3] Aghababaei, R., Warner, D. H. & Molinari, J.-F. Critical length scale controls adhesive wear mechanisms. *Nat. Commun.* **7** (2016).
- [4] Aghababaei, R., Warner, D. H. & Molinari, J.-F. On the debris-level origins of adhesive wear. *Proc. Natl. Acad. Sci.* **114**, 7935–7940 (2017).
- [5] Aghababaei, R., Brink, T. & Molinari, J.-F. Asperity-level origins of transition from mild to severe wear. *Phys. Rev. Lett.* **120**, 186105 (2018).

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