Simulations of sliding contact at the nanoscale: evolution of roughness

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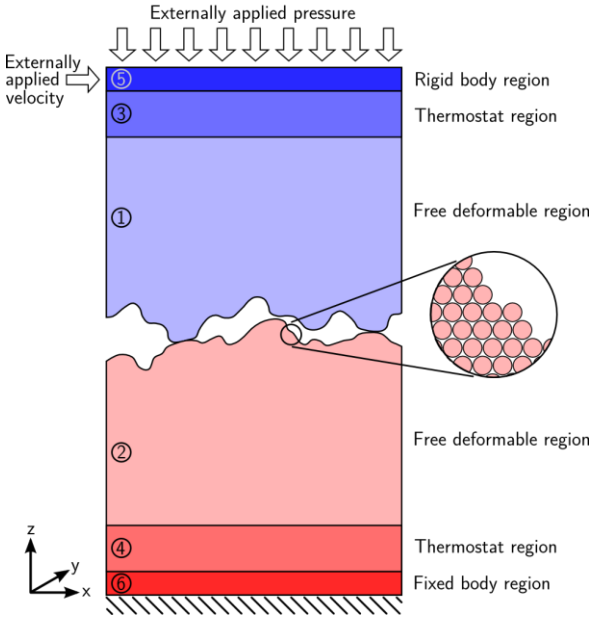
Tribological problems are particularly difficult to comprehend. Different physical mechanisms (including environment, plastic deformation, third body interactions, phase transformations, recrystallization) interact at disparate length scales. In this presentation we will illustrate some of our recent attempts to understand some of the molecular mechanisms at the origin of friction.

We begin with molecular dynamics simulations of dry sliding contact between rough solids, see figure. The roughness is created with a self-affine fractal model. For the case of a ductile (metallic) model material, we show that roughness is strongly altered during sliding motion and we evidenced a surface flattening that follows an exponential decay and reduces the friction to almost zero. However, recent simulations reveal that more complex mechanisms appear if we increase the brittleness of our model material. Brittleness generates micro cracks, which in turn create third bodies, increasing the overall roughness of the contact surfaces. Finally, we discuss our ongoing efforts at modeling a third body exhibiting fluid-like properties, which dissipates sliding energy and protects asperities against wear. The third body takes the form of a polymer fluid in the interstitial volume between the bodies. When a third body is included, large deformations prevent the computation of a friction coefficient by a direct measure of the forces acting between the two solid bodies. We developed a technique that correlates the total dissipation of the system, controlled with the work done by the thermostats, with a measure of the friction itself. After validating the approach, we discuss surface roughness evolution in presence of lubricant.



Schematic of 3D dry sliding contact
between rough solids