Load-dependent real contact area at nanoscale

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The real contact area introduced by Bowden and Tabor in 1939, is nowadays a widely used concept to quantitatively describe friction, lubrication, and wear at various length scales, and

"*The real area of contact is not greatly affected by the size, shape and degree of roughness of the surface: it depends mainly on the pressure. The general behaviour is consistent with the view that the surfaces are held apart by small irregularities*." [1] – called asperities

It is also well known that the contact models developed over the last decades for macroscopic bodies [2] fail to provide the real contact area at nanoscale. [3]

Matter of contact

Using classical molecular dynamics (MD) data, for example, is very challenging to define and estimate the load-dependent real contact area $A_{asp}(L)$ occurring due to the nanoasperities – see Fig. 1.

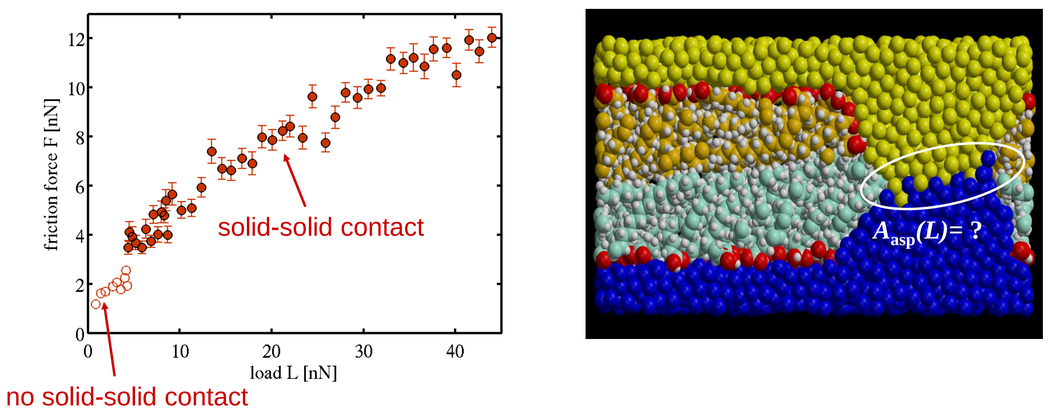


Fig. 1: Friction-versus-load behaviour (left) obtained in classical molecular dynamics simulations for a nanoscopic system consisting of two Fe substrates with a semi-spherical asperity, (yellow and dark blue) and covered by stearic acid (right); other colours: carbon (top/bottom) orange/light blue, hydrogen white and oxygen red. [4]

Therefore, one of the major issues to be dealt with, when estimating $A_{asp}(L)$ in MD, is the mapping of the discontinuous (atomic) view of matter onto a continuous one.

Contribution of smoothed atoms

This task is solved with our post-processing numerical tool, [5] by replacing the punctiform atoms with smoothed particles differentiated via their radii and smoothing lengths. Thus, the nanotribological system of interest turns into an ensemble of continuum media, which allows one to uniquely identify and realistically determine all atomic contributions to the load-dependent real contact area – see Fig. 2.

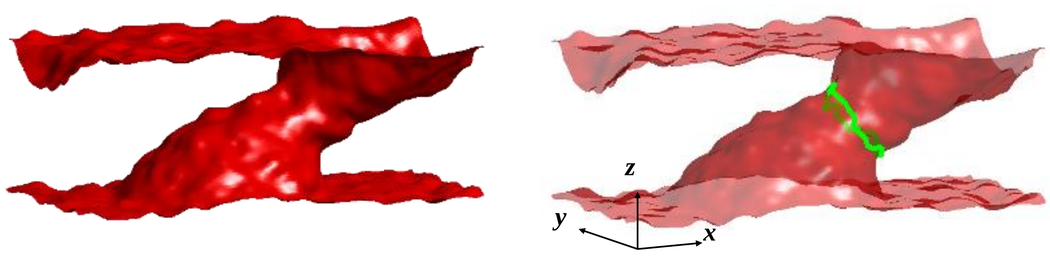


Fig. 2: Smoothed-atom representation of Fe-surfaces in Fig. 1 (left). The green line contours $A_{asp}(L)$ by connecting the closest non-Fe points in all considered 2D slices of contact zone (right).

With the so resulting $A_{asp}(L)$, classical MD simulations revealed that a **three-term kinetic friction law** (3-TKFL)

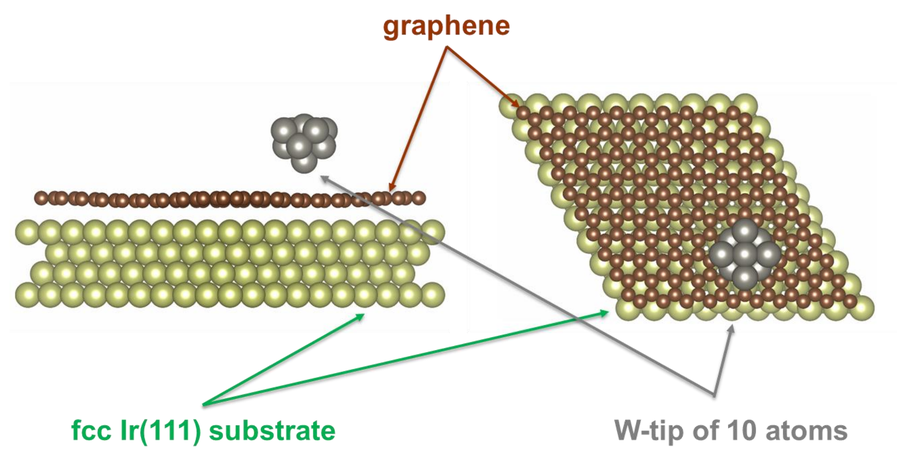
$$F(L) = F_0 + \tau A_{\mathrm{asp}}(L) + \mu L$$

entirely explains the friction-versus-load behaviour in mixed- and boundary-lubricated nanoscopic tribological systems, and even within the transition between these two lubrication regimes. [6]. It is remarkable that this 3-TKFL besides of the Bowden-Tabor adhesion-controlled term $\tau A_{asp}(L)$ and the Amontons-Coulomb load-controlled term μL, contains also a load-independent Derjaguin-offset F_0 which together with the shear strength τ and the coefficient of friction μ, form a complete set of independent constitutive system parameters.

Contribution of electrons

The Bader-partition [7] of the electronic charge density obtained using a van-der-Waals density-functional theory (vdW-DFT), [8] it is shown that directly permits the *ab-initio* calculation of the load-dependent contact area, i.e., the completely parameter-free determination of $A_{asp}(L)$ at nanoscale. [9] Since the Bader-atoms are limited in space by the zero-flux surface of the electronic charge density gradient field around the nuclei, in our computational scheme, the jump-to-contact of the interacting atoms unambiguously indicates the occurrence of a non-vanishing real contact area.

For a tungsten tip approaching graphene on an iridium substrate,



it was found that the *ab-initio* real contact area

- decays exponentially with the distance d_s between the tip apex and the carbon atom immediately below this, and
- its shape is mainly dominated by the symmetry of the graphene, but depending on the distance, it can be also influenced by the arrangement of atoms within the tip – see Fig. 3.

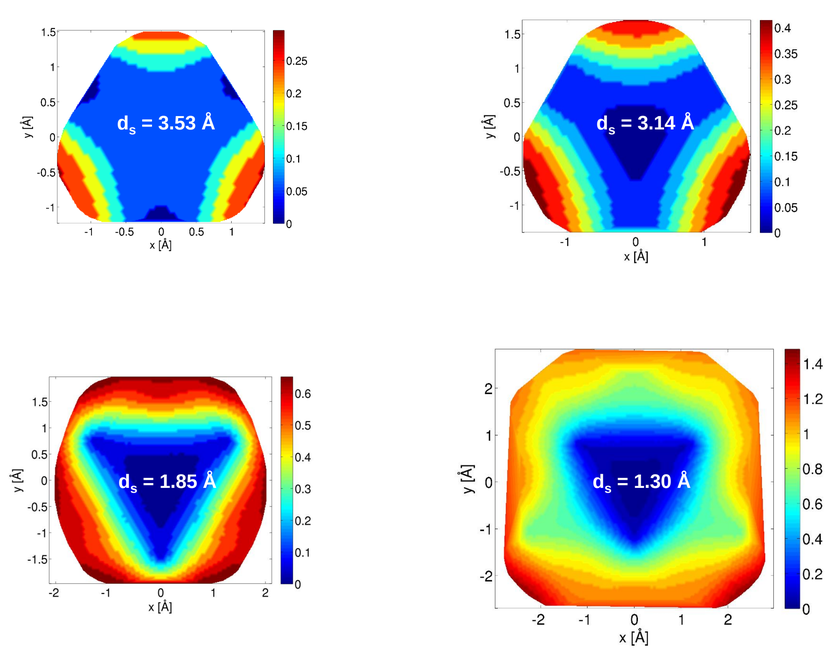


Fig. 3: Ab-initio real contact area calculated for four distances d_s between the tungsten tip and graphene on iridium. Different colours denote different heights from zero to 0.3 Å for d_s = 3.53 Å, and to 1.4 Å for d_s = 1.30 Å, respectively.

References

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Acknowledgement

This work was funded by the "Austrian COMET-Program" (project XTribology, no. 849109) via the Austrian Research Promotion Agency (FFG) and the Province of Niederösterreich, Vorarlberg and Wien and has been carried out within the "Austrian Excellence Centre of Tribology" (AC2T research GmbH).