Introduction

γ: surface energy

G: shear modulus σ*j* : shear strength

[1] R. Aghababaei, D. H. Warner & J.-F. Molinari. Critical length scale controls adhesive wear mechanisms. Nature Communications 7, 11816 (2016). [2] S. Pham-Ba, T. Brink & J.-F. Molinari. Adhesive wear and interaction of tangentially loaded micro-contacts. arXiv:1907.08183 (2019).

References

 $(1 - v)$ 2)*BN*² *d* 2 *q* 2 Elastic energy (*N* uniform loads) [2]

 $\overline{\mathcal{M}}$

plastic smoothening

failure involves the **creation of new surfaces**. To detach a semi-circular particle of diameter *d*, two surfaces of area *B*π*d*/2 have to be created, which requires an adhesive energy of $E_{ad} = \pi \gamma Bd$.

Objective - An analytical theory for the **interaction of multiple microcontacts** is derived in 2D, predicting the transition between a mild wear regime (formation of separate wear particles) and a severe wear regime (combined wear particles) at the scale of the micro-contacts.

THEORETICAL MODEL------

The formation of debris particles is possible if the stored elastic energy is greater than the adhesive energy required to create the particles, or in otherwords, if the energy ratio R is larger than one.

Adhesive wear and interaction of tangentially loaded micro-contacts

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Micro-contacts are modeled by*N***uniform loads** of magnitude *q* acting on a semi-infinite solid of thickness *B*. Only the bottom solid is considered because of symmetry.

Elastic energy

 $\mathcal{R} =$ *E*el *E*ad π*E*

- *E*: Young's modulus
- ν: Poisson's ratio
- γ: surface energy
- *d*: micro-contact size
- λ: micro-contact spacing

*d*a: aparent contact size

Adhesive energy

 $E_{el,Nq}$ =

The creation of a debris particle under a micro-contact assuming brittle

Three different outcomes from two sheared micro-contacts. The colors show the first principal stress σ_1 in reduced dimensionless Lennard-Jones units.

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The tribological interaction between two rough surfaces comes down to the contact of microscale asperities, forming micro-contacts. Recent work [1] demonstrated the existence of a **critical asperity size** *d* ∗ governing a **dutile-to-brittle transition** for a given material in an adhesive wear situation. A *single* micro-contact of size *d* will plastically deform under shear if $d < d$
Objective - An ana ∗ , or create a wear particle if *d* > *d* ∗ ابا
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Validation using simulations

Energy criterion for debris formation

In a 2D semi-infinite medium, M is infinite. In a 2D system of finite size, M is finite but depends on the size of the system. In a more realistic 3D system, E_{el} is independent of system size.

separated wear particles combined wear particle

Quasi-2D MD simulations of sheared perfect junctions were performed to check the validity of the predictions for debris formation. A model pair potential was used [1].

Simulations near the $d_r = d$ ∗ dashed line show effects of the finite size of the system, neglected in our model. The other simulations with $N = 2$ and $N = 3$ are in good agreement with the predictions. Separated debris particles can form even in the "combined" region because it consumes less energy, which is not predicted by our model but expected. *d*r

Molecular dynamics

• We derived and validated a**wearmap**for the **formationof separated**

or combined debris particlesin an adhesive wear regime at the microscale.

- The **emergence** of a regime of **severe wear** can be physically explained by the energetic feasibility of forming combined debris particles under multiple micro-contacts.
- Future work will generalize these findings in a 3D setting (fractal rough surfaces).

• separated debris particles:
$$
R_{sep} = \frac{E_{el, Nq}}{E_{ad, sep}} = \frac{d_r}{d^*} \rightarrow d_r \ge d^*
$$

\n• combined debris particle: $R_{comb} = \frac{E_{el, Nq}}{E_{ad, comb}} = \frac{d_r^2}{d_a d^*} \rightarrow d_a \le \frac{d_r^2}{d^*}$

Conclusion

Distribution of the MD simulations on a wear map of the different outcomes of the system. The two dashed lines represent the theoretical debris formation criteria. White-filled and color-filled symbols represent simulations with sharp corners and rounded corners respectively.

With *N* = 1, we get the system's critical length scale: *d*

∗

=

 π

2

 $(1 - v^2)q^2 M$

γ*E*

With *^N* > 1, we get the **criteria for debris formation**:

