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Comparison between experimental and computational adhesive contacts

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Contact mechanics simulations of the past few decades have provided a lot of insight into the effect of roughness on adhesion, using a variety of different modeling approaches. However, the most accurate computational methods are usually not suited to simulate realistic surface dimensions and interactions, which would require an appropriate representation across many length scales and consequently imply prohibitive simulation times. This contribution aims to overcome some of the often overlooked or underestimated challenges in order to develop a simulation approach that is comparable to real-world experiments and capable of making reliable predictions in technological applications.

Keywords: contact mechanics, nominally flat surfaces, multi-scale modeling, virtual experiment

1. Introduction

Modeling adhesive hysteresis is a computationally demanding task because its proper description requires short-range adhesion to be used, which leads to stiff differential equations. In this work, new approaches are described with which the efficiency of contact-mechanics simulations is increased so far that comparisons to experiments probing adhesive hysteresis, contact area and pull-off force become possible. This will ultimately be used to make reliable real-life contact predictions for practical pick-and-place applications.

2. Methods

In the spirit of the contact-mechanics challenge [1], we investigate systems consisting of a soft, semi-infinite elastomer, which is in adhesive contact with a stiff indenter of defined microroughness. However, we do not only simulate artificially generated surfaces, but also real topographies that have been imaged via laser scanning microscopy (LSM).
The Green's function molecular dynamics (GFMD) simulation approach [2] has proven to be successful for the simulation of periodically repeated small sections of randomly rough surfaces. If a non-periodic macroscopic specimen geometry is simulated, the effect of periodic boundary conditions (PBCs) needs to be counteracted, for example by padding the surface as in Figure 1a. Unfortunately, this voids the otherwise beneficial effect of PBCs that (infinitely) large surfaces can be represented by a small simulation cell. Therefore, the GFMD code needs to be refined and enhanced to efficiently run realistic simulations.
Multiple approaches are tested and compared. Apart from further optimizations to surface interaction and relaxation dynamics, the length scale dependence is analyzed with the goal to develop a multi-scale approach: A cohesive-zone model (CZM) will be constructed from the bottom up. In a first step, only the interaction on the small scales is simulated and then transferred to other simulations at coarser scales.

3. Results and discussion

The main computational difficulty is to model the much-neglected approach-to-contact dynamics, as microscopic asperities jumping into contact set the most stringent requirements on the range of adhesion to be used in the simulations. We have found that a value below 10-20 % of the rms height is usually needed to obtain realistic hysteresis and preload dependencies.
Figure 1 shows a brute-force simulation of a whole pillar with a diameter of 1.5 mm. The magnified view shows how a single macroscopic contact region consists of many individually adhesive and repulsive asperities depending on approach and retraction, contributing to the hysteresis in the load-displacement curve.
Since real surfaces are only self-affine up to a maximum wavelength λ, first results show that a reasonable estimate of the pressure-displacement curve can often be obtained modeling only an area of lateral dimension in the range of ~2-4λ. This makes the CZM approach in development look very promising for practical applications with much shorter simulation times.

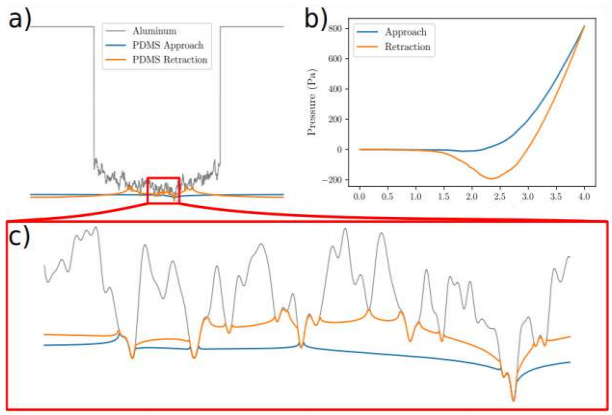

Figure 1: Simulation of an aluminum pillar sticking to a PDMS substrate. a) and c) show the cross-section of the contact geometry for approach and retraction at the same macroscopic displacement of 2 µm. b) shows the obtained load-displacement curve.

4. References

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