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# Nano-scale roughness effects on hysteresis in micro-scale adhesive contact

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ABSTRACT

A multi-scale model enables investigation of the effect of surface roughness on energy loss in adhesive contact. Fully atomistic simulation of nano-scale indentation predicts size-dependent force–distance trends that are introduced as roughness into a micro-scale finite element model through randomly distributed non-linear hysteretic springs. The multi-scale model predicts that the energy loss, quantified by the hysteresis loop formed by loading and unloading data, increases with increasing indentation depth and surface roughness. This behavior is discussed in terms of an analytical model of a simply connected system.

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## 1. Introduction

Adhesive contact plays an important role in a variety of tribological applications. One such application is a micro-electro-mechanical systems (MEMS)-based switch. MEMS switches can be smaller and faster than currently employed mechanical relays and so have significant potential for many low-power applications; however, they are limited in their usefulness by issues with deteriorating performance and failure associated with adhesion between the contacting components [1]. There is, therefore, significant potential benefit to understanding adhesive contact and how it might be controlled through design or during operation.

Analytical and numerical modeling of adhesive contact between rough surfaces is by no means a new area of research. Early work by Greenwood and Williamson [2], Johnson, Kendall and Roberts [3], and Derjaguin and Müller–Toporov [4] has been the foundation of many subsequently reported continuum model-based studies (see for example [5–8]). Adhesive contact on much smaller length scales has been studied using molecular dynamics (MD) simulation (see for example [9–12]).

However, the critical interface behavior of a MEMS switch is affected by both the micro-scale contacting body and the nano-scale asperities. This is potentially an issue since the discrete behavior of the nano-scale asperities may not be captured by a continuum theory, while the micro-scale contact is too large to be described using atomistic methods. Therefore, length scales range from atomic to tens or hundreds of microns which suggest that multi-scale models are necessary to capture the relevant physics. Recent examples of multi-scale, rough surface contact models are a local quasicontinuum method [13], Hertz elasticity applied to hierarchical roughness [14], course-grained molecular dynamics simulation [15], and hybrid models combining MD and finite element methods (FEM) [16,17]. Closely related to this work, Eid et al. [18] reported a multi-scale model that used the force–displacement data from MD simulation of nano-scale indentation to describe the behavior of individual asperities on the surface of a micro-scale body.

Here, we use an approach similar to [18] as a base, but significantly extend both the method and the analysis by introducing randomly distributed asperity sizes to vary roughness, and focusing on depth-dependant hysteresis and associated roughness-dependent energy dissipation. We developed a 3D multi-scale approach combining an FEM model of a micro-scale contact using Abaqus with an MD model of nano-scale roughness. The MD-predicted force–displacement behavior is introduced into the FEM model through non-linear, hysteretic springs with randomly distributed heights where the spring response to deformation is determined from linear interpolation of MD data. We investigate the energy loss (hysteresis between loading and unloading) both at the single asperity and multi-asperity rough surface scales. The model predicts that energy loss is affected by roughness and indentation depth and we analyze these finding in terms of a simplified model of wavy surface elastic contact.

## 2. Methodology

In this research we define two separate length scales to capture the tip of the MEMS contact and the roughness of that contact. We assume that the larger scale contact is on the order of

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microns and the roughness is on the order of nanometers. The former is modeled using finite element analysis and latter using atomistic simulation. Details of these two methods and their integration into a multi-scale model will be given in the following sections.

### 2.1. Atomistic simulation

Molecular dynamics simulation is used to capture the atomic-scale mechanics of single asperity contact. The model consists of a hemisphere (asperity) indenting the (111) face of an atomically flat surface (block). A snapshot of the model is shown in Fig. 1. There are three model hemispherical asperities having radii of 2.217 nm, 3.050 nm, and 3.881 nm. Periodic boundary conditions are applied along the $x$–$y$ plane with a free boundary condition in the $z$-direction (direction of indentation). The bottom three layers of the asperity are fixed and the top three layers of the block are treated as a rigid body. All atoms are modeled as Platinum with interatomic interactions described by the Embedded Atom Method (EAM) [19] with Pt-specific parameters [20].

The block is initially placed a distance greater than the cutoff of the potential ($r_{cut} = 0.56$ nm) from the peak of the hemispherical asperity so that there is no interatomic force. The system is equilibrated in the NVT (constant number of atoms, volume, and temperature) ensemble at 300 K (Nosé–Hoover thermostat) for 40 ps and then in the NVE (constant number of atoms, volume, and energy) ensemble for another 40 ps. We observe that the temperature and potential energy are stable during the NVE ensemble stage and so infer that the system has reached thermal equilibration.

There are two stages after the equilibration process, loading and unloading, both of which are run in the NVT ensemble at 300 K. The rigid layers of atoms at the top of the block are moved with a constant velocity of 1 m/s towards the asperity in the loading stage. The block is moved downward until it reaches its maximum approach where the approach is defined as the distance between the initial height of the asperity and the average $z$-position of the atoms in the bottommost layer of block. With this definition, the approach is negative at the onset of loading, and then becomes positive once the asperity and block are in contact. Three different simulations with different maximum approach are run for each asperity size. Asperity radius 2.217 nm is run to 0.5, 1.1 and 1.4 nm, asperity radius 3.050 nm is run to 0.5, 1.2 and 2.0 nm, and asperity radius 3.050 nm is run to 0.5, 1.5 and 2.7 nm. After the block reaches the maximum approach, the rigid body atoms are assigned an upwards velocity of 1 m/s to simulate unloading. The simulation is stopped after the block completely detaches from the asperity. The approach and the interaction force are tracked throughout the entire process, where the force is calculated as the sum of the interaction force between atoms in the asperity and atoms in the block. Because there is some atom transfer between block and asperity, this method of calculating force is not exact. However, experimentation with multiple means of force calculation (for example, identifying the separation between asperity and block as the location of the smallest cross-sectional area of the continuous neck connecting them) reveal that the effect of this detail in the force calculation method has a negligible effect on the predictions of the multi-scale model which will be discussed next.

### 2.2. Multi-scale model

Abaqus is used to create a three-dimensional, continuum model of a micron-scale (radius 1 μm) hemispherical platinum tip using HyperMesh to create the finite element mesh. A snapshot of the model is shown in Fig. 2a. Young's modulus, Poisson's ratio and ideal yield strength are taken to be 168 GPa, 0.3 and

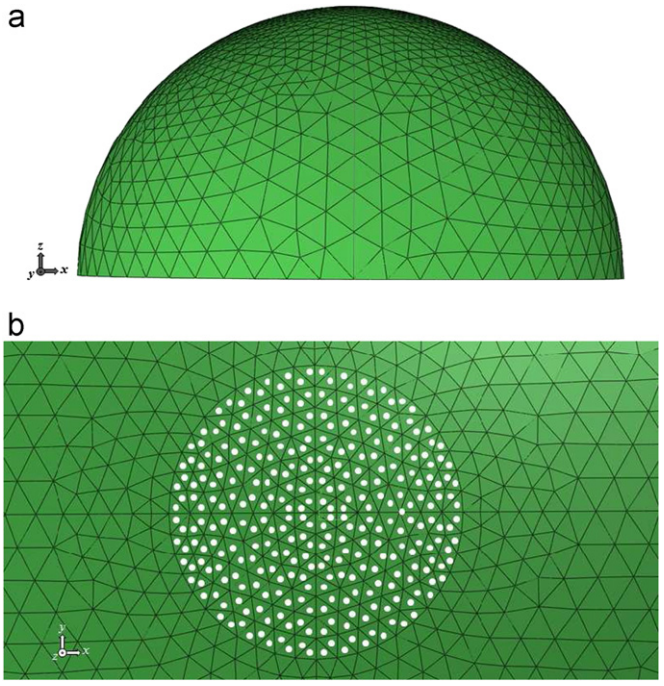


**Fig. 2.** Finite element model of a hemispherical contact; (a) perspective view and (b) top view identifying the potential locations of MD-modeled asperities.

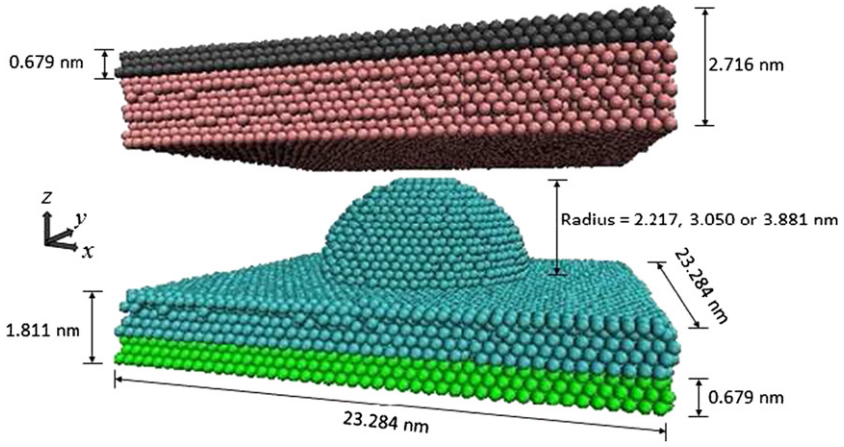


**Fig. 1.** Snapshot of the molecular dynamics simulation of nano-scale asperity contact.

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