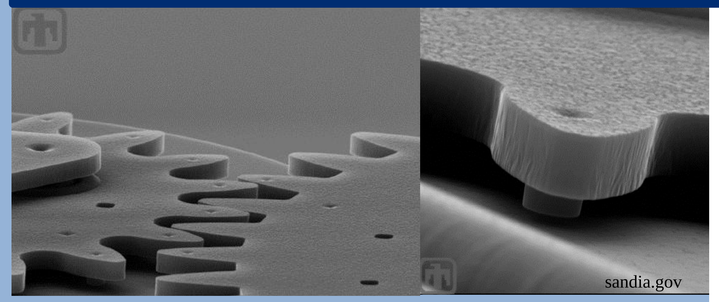
Scale effects in static friction between rough solids

Tristan A. Sharp, Lars Pastewka, Mark O. Robbins

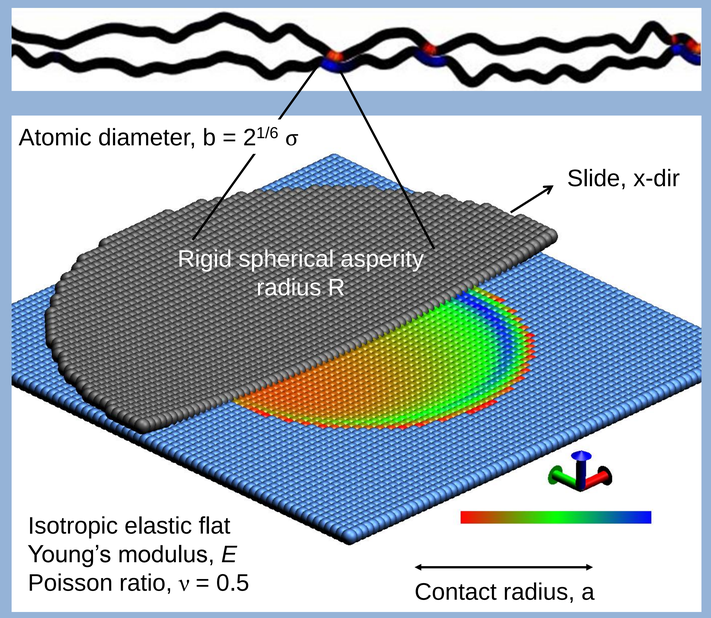
JOHNS HOPKINS UNIVERSITY

NSF idies The Institute for Data Intensive Engineering and Science



Introduction

Understanding small-scale deformation and energy dissipation between contacting solids is important in applications that range from nanoscale mechanical devices to jet engines. Even finely-smoothed parts exhibit roughness, and contact between solids generally occurs only at asperities, often approximated as spheres. Here, we use molecular dynamics simulation to investigate sliding of a single asperity and to identify scale effects of the static friction coefficient, μ.



We simulate the quasistatic sliding of an asperity composed of a bent lattice, choosing the lateral spacing of the surface atoms to be commensurate with the lattice of the substrate. Repulsive Lennard-Jones (LJ) interactions produce a square (x-y) lattice of atomic corrugations. The substrate is controlled by the Green's function of isotropic linear elasticity[4].

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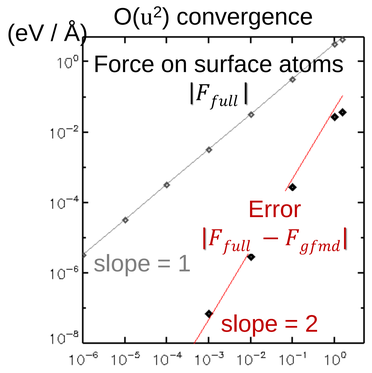
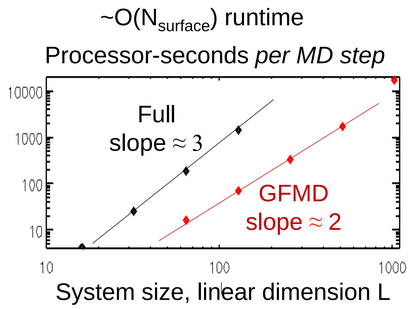
References:
1 JA Hurtado and Kim. Proc. R. Soc. Lond. A. 1999 1471-2946
2 Yanfei Gao J. Mech. Phys. Solids 58 (2010) 2023-2032
4 L. Pastewka, T. Sharp, M. O. Robbins. PRB 86 075459 (2012)
5 S. Plimpton. J Comp Phys, 117, 1-19 (1995)

Method: Molecular Dynamics and Greens Function - MD

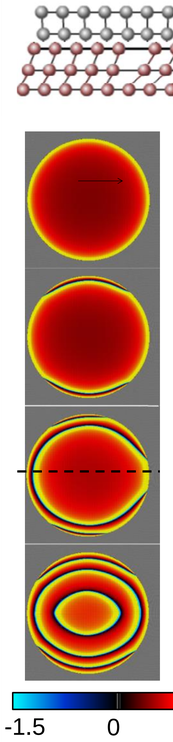
To study large systems, we helped develop a parallel, multi-scale simulation package which accelerates molecular dynamics simulation. The acceleration is achieved by replacing part of a solid with its Greens function response. The method requires calculating the energy about a reference state and Taylor expanding to second order in the atomic displacements, u. Once the Greens function is calculated, calculations can be performed quickly, scaling with the number of atoms on the surface of the solid, $N_{surface}$.

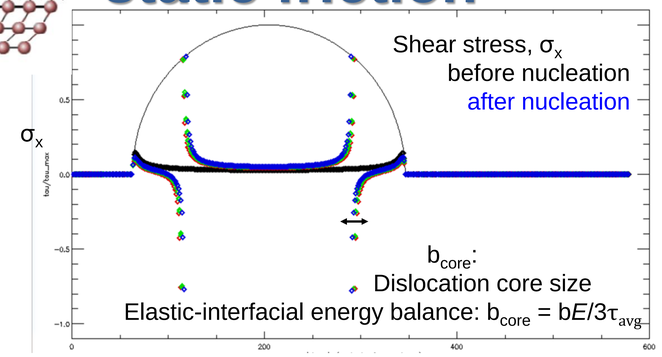




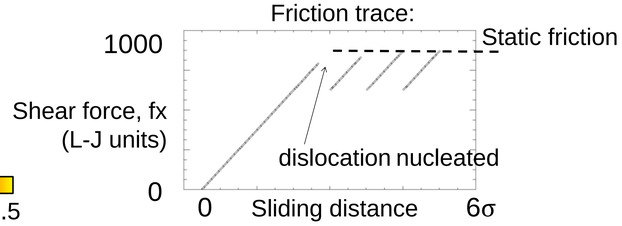
Also, implemented on GPU. Also, fewer atoms means shorter convergence time

Dislocations decrease static friction

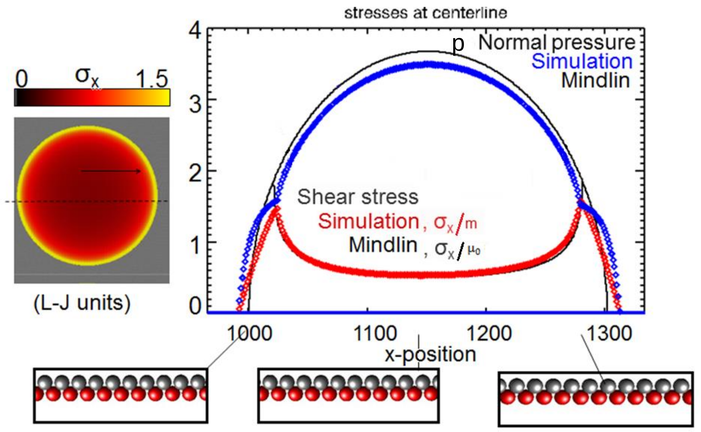




If a>b_{core}, the sphere need not overcome the corrugation stress all at once. Nucleation of a dislocation results in partial slip. Dislocation annihilation at the center moves the contact one Burger's vector, b.

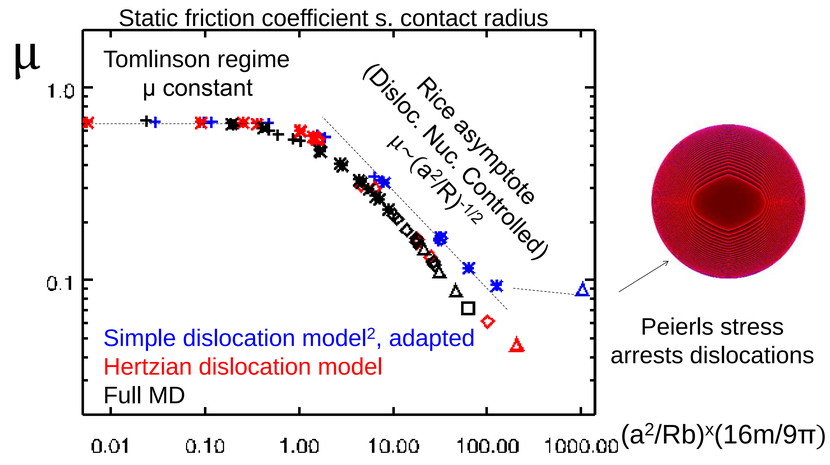


Contact Stresses



Shear stresses at the edge cannot exceed the normal pressure, p, times the corrugation max slope, m. This explains the correspondence with the Mindlin continuum model (which uses Hertz pressure and a local friction coefficient, μ_0). In the simulations, atomic corrugation slope mimics the role of μ_0. Applying sufficient stress causes the sphere to coherently hop one atomic diameter..

Scale effects in friction



Small contact regime: static friction requires overcoming corrugation stress (m x pressure) over the full contact area.
Large contact regime: friction drops as $(a^2/R)^{-1/2}$ due to contact edge stress maximum nucleating dislocations.
Very large contact regime: Peierls stress dominates