# Multiscale Modeling of Stiffness, Friction and Adhesion in Mechanical Contacts

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## Defining Contact at Atomic Scales

### STATUS QUO

**Macroscopic Theories Assume Stiffness, Friction and Adhesion Scale with Real Contact Area $A_c$**

• Friction proportional to $A_c$ and $A_c$ proportional to load L for rough surfaces • Flat surfaces in complete contact at any load

**Molecular Simulations Differ on Applicability of Macroscopic Results at Atomic Scales**

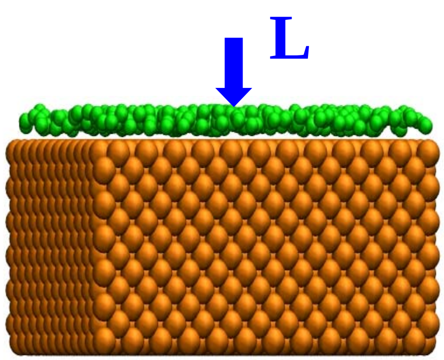
•Linear scaling of $A_c$ with load in some cases

• Strong variation with atomic scale roughness in others

### NEW INSIGHTS

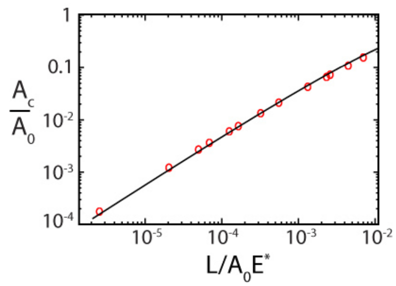
**Atomic Scale Contact is Different**

• Atomic simulations of flat surfaces allow simple contrast with continuum models • Macroscopic models assume that flat surfaces have full contact at any finite load • Thermal fluctuations may profoundly affect contact at atomic scales



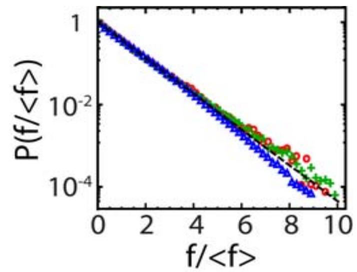

Flat amorphous surface and elastic substrate

### MAIN ACHIEVEMENTS:




Fraction of surface atoms in contact, $A_c/A_0$, as a function of load, L, for flat amorphous surface. $A_0$ is nominal area, E* is modulus. Line is analytic theory

• Different atomic scale geometries exhibit universal contact behavior • Instantaneous force on atoms has exponential distribution (below) • Fraction of atoms in contact rises linearly with load (above) • Transition from no contact to full contact for flat surfaces is not sharp ⇒ Occurs over pressure range comparable to ideal yield stress • Simple analytic theory ⇒ quantitative description




Probability of local force f normalized by mean force <f> shows universal exponential distribution. Load $L/A_0E^*=2\times10^{-5}$ (o), $5.5\times10^{-4}$ (+) and 0.007 (Δ)

### HOW IT WORKS:

• At typical temperatures, thermal pressures are surprisingly large compared to yield stress • Atoms vibrate in and out of contact • Small fraction of time in contact supports large load

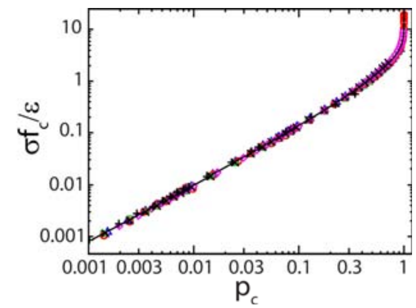
### ASSUMPTIONS AND LIMITATIONS:

• Calculations use simple generic pair potentials, but analytic model allows generalization to arbitrary materials

### QUANTITATIVE IMPACT

**Current Impact**

• Results raise questions about meaning of $A_c$ and assumed connection to stiffness, friction and adhesion in macroscopic models • Results for flat surfaces can be mapped directly to other geometries using universal relation between force and time in contact




Universal curve for mean force on atom $f_c$ and fraction of time in contact $p_c$ for flat and spherical tips with amorphous and crystalline surfaces (different symbols). Line is analytic theory.

**Planned Impact**

•Develop new relations between $A_c$ and stiffness, friction, and adhesion of rough surfaces that incorporate effect of thermal fluctuations

### END-OF-PHASE GOAL

**Research Goals**

• Models of contact and stiffness of multiasperity contacts that bridge from atomic to macroscopic descriptions • Predictive models for mechanical properties of single and multi-asperity contacts