Multiscale Modeling of Stiffness, Friction and Adhesion in Mechanical Contacts
Mark O. Robbins --- FA9550-0910232

Defining Contact at Atomic Scales

Macroscopic Theories Assume Stiffness, Friction and Adhesion Scale with Real Contact Area $A_c$
- Friction proportional to $A_c$ and $A_0$
- 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

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

MAIN ACHIEVEMENTS:
- 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

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.

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

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

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

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

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

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

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.