MAR16-2015-004453

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Spanning From Atoms to Micrometers in Simulations of Contact, Adhesion and Friction[1]

MARK ROBBINS, Johns Hopkins University

Improved understanding of the forces between realistic solid surfaces is needed to optimize adhesion and friction. Modeling these forces is challenging because they arise from interactions between atoms separated by less than a nanometer, but the number and spatial distribution of these contacting atoms depends on surface roughness and deformation on micrometer and larger scales. There are also strong scale effects in the role of elastic deformations along the surface. The talk will first describe a seamless Greens function (GF) method that allows a full treatment of elastic deformations and atomic contact for micrometer scale surfaces and multibody potentials. Next applications of the method to calculations of the contact area, contact stiffness, adhesion and friction for a range of geometries and interactions will be described. The results can be captured with simple analytic expressions and explain why most contacting surfaces do not adhere. Theoretical and experimental studies of single nanometer-scale asperities show that the frictional shear stress depends strongly on whether surfaces are commensurate. A large constant stress is obtained for identical, aligned crystalline surfaces, but the stress averages to zero in the more common case of incommensurate surfaces. The resulting ultralow friction is called superlubricity and is found in experiments and simulations of small contacts. Our simulations reveal dramatic changes in this behavior because different parts of the surface are able to advance independently as the contact radius increases towards micrometer scales. The friction between identical surfaces drops with increasing radius and then saturates at a low value. The force between incommensurate surfaces saturates at a similar value that can be related to the Peierls stress for dislocation motion at the interface. Studies of multiasperity contacts also show that incoherent motion along the interface can lead to pronounced changes in the macroscopic friction.

[1]This material is based on work supported by National Science Foundation Grant DMR-1411144.