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Effects of atomic-scale geometry in contact of rough surfaces[1]
TRISTAN A. SHARP, LARS PASTEWKA, MARK O. ROBBINS, Johns Hopkins University — There has been great recent progress in continuum models of the effect of roughness on the area, friction, and stiffness of contacts between two solids. This talk will use molecular dynamics simulations to study how atomic scale features on surfaces can affect contact properties. Beginning from the established case of continuum linear elasticity that gives a linear relationship between real contact area and load, we systematically introduce atomic-scale physics to determine the affects on contact. Replacing an ideal linear isotropic elastic medium with a harmonic atomic lattice produces only small changes in the mechanical response. For more realistic interactions, anharmonicity and plasticity typically increase the contact area. The atomic steps present on rough crystal lattices lead to increased plasticity and change the small scale structure of contacts. Depending on the tendency for the material to yield, the presence of steps can increase or decrease the area of very high pressure, but steps always decrease the area of very low pressures. The large scale structure of the contact is the same for all cases. Application of continuum contact theories to surfaces with atomic-scale features will be discussed.

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