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When does continuum theory describe mechanical contacts?[1]

BINQUAN LUAN, MARK O. ROBBINS, Johns Hopkins University — Continuum theories of contact assume that discrete atomic displacements can be described by continuously varying strain fields and also that surfaces are perfectly smooth at small scales. While the first assumption is know to fail as dimensions decrease to atomic scales, continuum results are routinely applied to atomic force microscope tips and other nanoscale contacts. We have used molecular simulations of contact between a rigid sphere or cylinder and a flat elastic half space to test the limits of continuum theory. The flat surface was a (100) or (111) surface of an fcc crystal. Tips were made by bending perfect crystals to a radius of curvature R, or cutting surfaces of mean radius R from crystals or amorphous solids. The normal displacement vs. load curves for all tips are close to continuum predictions, as are extracted elastic moduli. Local quantities such as the width of the contact and local pressures can vary by more than a factor of two from continuum predictions. Friction forces and lateral contact stiffnesses vary by at least an order of magnitude with atomic scale geometry. Analysis of these results shows that the assumption of smooth surfaces is a greater source of error than use of continuous strain fields.

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