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Contact of rough surfaces at the atomic scale TRISTAN SHARP, Johns Hopkins University, LARS PASTEWKA, Fraunhofer Institute for Mechanics of Materials IWM, MARK O. ROBBINS, Johns Hopkins University — Roughness on solid surfaces typically causes contacting solids to remain microscopically separated, with important consequences for sealing, adhesion, and friction. Continuum theory and continuum simulations of rough contact have greatly contributed to a statistical understanding of these processes. However, continuum treatments neglect atomic-scale geometry at the surface, thereby making an uncontrolled approximation. Here, we perform molecular dynamics simulations of rough surfaces to test the consequences of atomic-scale features. We focus on atomic plasticity and atomic steps that form terraces on rough surfaces of crystalline solids. We find that the atomic features treated here do not dramatically alter the large-scale solid deformations predicted by continuum calculations. However, different behavior emerges at small scales. Continuum treatments underestimate the number of atoms with very low and very high stress. Step edges concentrate stress and change the small-scale morphology of contact patches. A new statistical quantity, the characteristic ratio of step height to step width, is found to be useful when extending continuum theory to treat atomic-scale steps. These results are discussed in context of the recent scaling theory of Persson.

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