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A MICROMECHANICAL DISLOCATION MODEL OF ROUGH SURFACE CONTACT PLASTICITY

Y.F. Gao
Division of Engineering, Brown University, Providence, RI 02912

ABSTRACT

Rough surface contact plasticity, especially at mesoscale and nanoscale, has been playing a central role in a broad spectrum of novel applications, e.g. nanostructure fabrication and reliability. The multiscale nature of surface roughness, the structure- and size-sensitive material deformation behavior, and the importance of surface forces and other physical interactions give rise to very complex surface phenomena at mesoscale and nanoscale. We present a micromechanical model to study rough surface contact plasticity, based on dislocation nucleation and multiplication. Surface roughness can be sources of dislocation nucleation; though roughness is confined to a thin layer, the resulted dislocation plasticity can extend to a far depth. Depending on interface adhesion, roughness features and slip planes, we get a variety of surface micro-plasticity behaviors that are radically different from classic plasticity behaviors.

INTRODUCTION

Surfaces of most engineering materials are unavoidably rough, and contain geometric irregularities (asperities) with feature sizes ranging from micrometers to nanometers.[1] Starting from a fractal description of surface roughness, several recent works[2,3] conduct the contact analysis from the long wavelength and refine the pressure and contact size distributions by adding more roughness scales according to the roughness spectrum. It is also shown that a perfectly fractal description of surface roughness appears to lead to unphysical predictions of the true contact size and number of contact spots, for both elastic and elastic-plastic solids, mainly because of the artifact of the ideal fractal property and the classic plasticity. Nevertheless, those models agree very nicely with extensive finite element simulations.[4]

However, regardless of numerous efforts in modeling rough surface contact, few works consider the importance of surface deformation properties at mesoscale and nanoscale. Surface failure phenomena are not determined by macroscopic contact nor is it determined on the atomic level. The microstructure- and size-sensitive deformation behaviors near and at the rough surface would be the critical link in this multiscale contact problem. For example, the material hardness is found to be size dependent at submicron scale.[5] We define *surface micro-plasticity* as the study of dislocation nucleation and pileup from the surface roughness, and the interaction between defects and novel surface properties and bulk defect microstructures. This line has not received sufficient attentions for the study of small-scale rough surface contact.

In this work, we study a stepped surface under adhesive contact, and examine the behavior of near-surface dislocation nucleation and pileup. Key results will be briefly reviewed.

SURFACE STEP CONTACT MODEL

When the stepped surface shown in Fig. 1 is pressed by a smooth rigid surface, the step can nucleate dislocations and its height decreases so the surface becomes smoother. In the standard continuum dislocation model, the dislocation is treated as an elasticity singularity, and the driving force on it can be calculated once the elastic field is determined. Various analytical and numerical methods can be used for this purpose. The “short-range” dislocation interactions are usually modeled by a set of constitutive relations, such as the conditions of dislocation annihilation, junction formation, dislocation nucleation etc. In this work, we adopt the well-known Rice-Thomson model[6] for the dislocation nucleation from a stress singularity. If the driving force on a fictitious dislocation (that is placed at distance η from the stress singularity, e.g. a crack tip or a step in this paper) is larger than an effective lattice resistance, i.e. the Peierls stress G_p, the dislocation will be nucleated. Those two parameters can be calibrated by atomistic simulations. The energetic driving force in conjunction with the Rice-Thomson criterion determines the nucleation and equilibrium distance traveled by the dislocation away from the surface step. And the effect of surface adhesion, step size and lattice resistance on our step-dislocation model can be easily studied.

Figure 2 presents the critical loads for dislocation nucleation at the slip plane L.[7] The interface work of adhesion

$\Gamma/c_{11}b$ (normalized by c_{11}, the elastic constant, and b, the magnitude of the Burgers vector) is 0.02. With a given step height h, dislocations can be nucleated one by one with the increase of the applied pressure σ^{∞} (negative means compression). The Rice-Thomson microstructural length is $\eta/b = 5$. The change of Peierls stress G_p only shifts those results, but does not change the conclusion qualitatively.

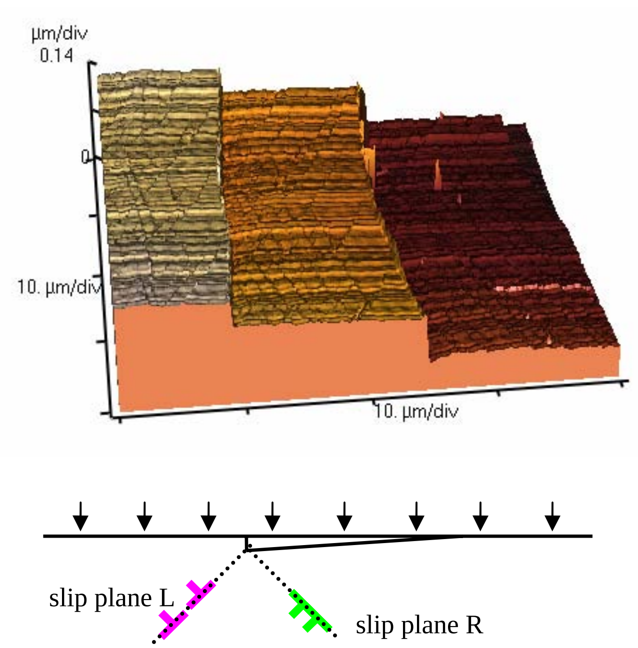

Figure 1 – An Atomic Force Microscope image of a cleaved LiF single crystal. The surface ledges, under contact, will emit dislocations along certain slip systems, as shown schematically.

Multiple dislocations can be nucleated and pileup near the rough surface, and usually form distinctive slip lines. We have found that nucleated dislocations generate back stress at the surface dislocation source, leading to surface hardening behavior (as in Fig. 2). The cooperative hardening between different slip planes can be order-of-magnitude weaker than the single-slip-plane hardening curve (results are not presented here). Multiple dislocation pileups and the cooperation between neighboring slip planes lead to a dislocation structure that cannot be predicted by the classic plasticity theory.

DISCUSSION

From the theoretical work reported here, we can establish a statistical model of rough surface contact based on the interaction between neighboring surface steps and between surface and bulk dislocation sources. Consequently, we can construct a scale-bridging model of small scale contact conformity and the interaction between adhesion and dislocation-based surface plasticity.

We can easily extend this model to study asperity friction. The classic stick-slip scenario[1] will be replaced by the introduction of dislocations from the contact edge. The competition between those interface dislocations and sub-surface dislocations will be a major mechanism for incipient asperity sliding at small scales.

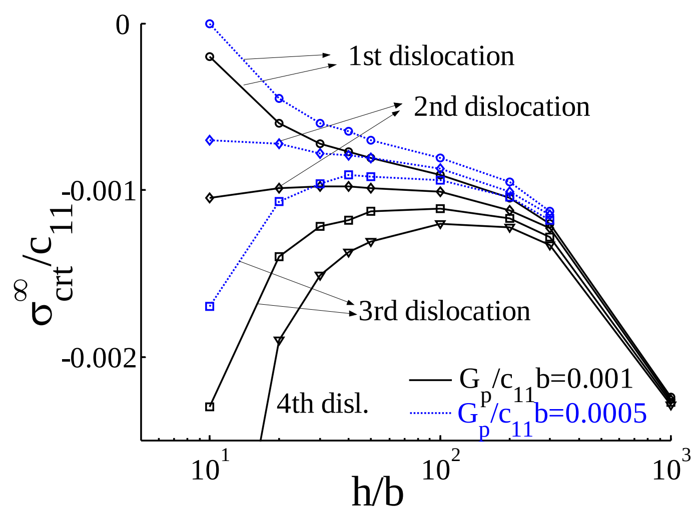

Figure 2 – Critical loads for dislocation nucleation are plotted against the step height h/b (normalized by b, the magnitude of Burgers vector). This plot only considers the slip plane L.

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