

Dislocation Nucleation and Segregation in Nano-scale Contact of Stepped Surfaces

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ABSTRACT

A myriad of engineering applications involve contact between two surfaces, which induces localized plastic deformation near the surface asperities. As a generic problem in studying nano-meter scale plastic deformation of solid surfaces, a unit process model of dislocation formation near a surface step under contact loading of a flat rigid surface is considered. The driving force on the dislocation is calculated using conservation integrals. The effect of surface adhesion, step size and lattice resistance on the dislocation driving force are analyzed in a continuum dislocation model, while the nucleation process is simulated atomistically. The driving force formula is used for a dislocation nucleation criterion and to get the equilibrium distance traveled by the dislocation away from the surface step. Results of the unit process model show that under a normal contact load dislocations nucleated in certain slip planes can only stay in a thin layer near the surface, while dislocations nucleated along other slip planes easily move away from the surface into the bulk material. The former dislocation is named anti-load dislocation and the latter dislocation is called pro-load dislocation. Embedded atom method (EAM) is utilized to perform the atomistic simulation of the unit-process model. As predicted by the continuum dislocation model, the atomistic simulations also indicate that surface adhesion plays significant role in dislocation nucleation process. Varying the surface adhesion leads to three different regimes of load-deflection instabilities, namely, just dislocation nucleation instability for no adhesive interaction, two distinct surface adhesion and dislocation nucleation instabilities for weak adhesive interaction and a simultaneous surface adhesion and dislocation nucleation instability for strong adhesive interaction. The atomistic simulations provide additional information on dislocation nucleation and growth near the surface steps. The results of dislocation segregation predict existence of a thin tensile-stress layer near the deformed surface and the results on the adhesion effect provides a cold-welding criterion.

INTRODUCTION

It is widely accepted that the roughness of two contacting surfaces plays a big role in the contact fatigue and wear processes. Many researches have related the surface roughness to wear rate [1-4]. In these studies, after a detailed description of surface profile and the estimation of contact area, a simplified way of losing mass was assumed and purely geometric considerations were utilized to derive the wear rate. The studies clearly demonstrate the effect of roughness on surface fatigue and wear. However, the mechanism governing the nano-meter scale surface roughness evolution and its influence on surface contact fatigue and wear were not clearly understood.

When two rough surfaces are brought together, many asperities are in contact. The size and distribution of the contact spots depend on the surface roughness and the applied load. Even in the absence of macroscopic plastic deformation, permanent damage can occur in small scales under the contacting asperities leading to changes in surface roughness after the removal of load. One mechanism for the roughness change is dislocation nucleation and motion near the surface.

For example, when a stepped surface shown in Fig. 1 is pressed by a smooth rigid surface, the step can nucleate dislocations and its height decreases making the surface smoother. If a dislocation source in the bulk of the material creates a dislocation loop under external pressure, one end of the dislocation loop may reach the surface and roughen the surface. The roughness evolution without surface diffusion is the result of the dislocation nucleation, accumulation, and annihilation activities at the surface.

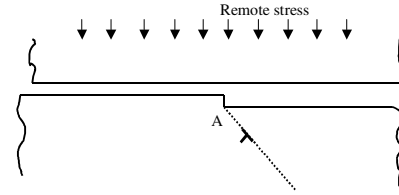


Figure 1 Roughness change due to dislocation nucleation

As a first step in understanding the surface roughness evolution, this paper examines a simple unit process: a metallic surface with only one surface step is subjected to a contact load by another rigid flat surface. A dislocation based multi-scale framework is developed to analyze the unit process model. Under contact load, a dislocation nucleates and grows out from the surface step. The driving force on the dislocation is calculated using conservation integrals. The effect of surface adhesion, step size and lattice resistance on the dislocation driving force are analyzed in a continuum dislocation model. The driving force in conjunction with the Rice-Thomson dislocation nucleation criterion [5] determines the nucleation and equilibrium distance traveled by the dislocation away from the surface step. Embedded Atom Method is utilized to perform atomistic simulation of the unit process model. The atomistic simulations are used to demonstrate the influence of the interaction between the indenter and the solid surface on the dislocation nucleation. The results of the atomistic simulations are utilized to determine the constitutive parameters associated with the continuum dislocation model.

UNIT PROCESS MODEL

The unit process (shown in Fig. 2) consists of a metallic surface with only one step indented by a rigid flat indenter. We assume the indenting surface is rigid, thus only the metallic stepped surface is studied for surface plasticity behavior. The indenter has a perfectly smooth surface so that when two materials are brought together, there is only one gap near the step. The width of the gap d is determined by the stiffness of the materials (C_{11}, C_{12}, C_{44}), the interface adhesion (Γ_{adh}), the remote load (σ_{22}^{∞}) and the step size (h). When load increases, the stress concentration near the step may nucleate a dislocation of Burgers vector b from the step, decreasing the step size to reduce the external potential. The dislocation nucleation criterion proposed by Rice and Thomson [5] is used to study dislocation emission from the surface step. Hence, if the driving force on a dislocation at a distance η from the step is greater than the Peierls force, the dislocation is emitted from the step. The Peierls force depends on the slip plane orientation (θ). Parameter η characterizes the size of the dislocation emission process zone near the step.

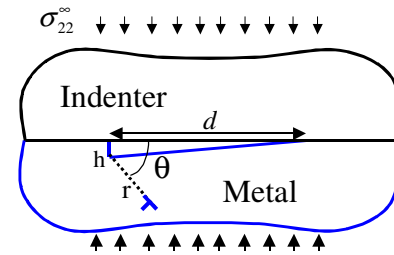


Figure 2 Schematic of the unit process model

The stress field associated with the unit-process model is determined by decomposing the main boundary value problem into linear superposition of the three sub-problems as shown in Fig. 3. Both the indenter and the metallic surface are assumed to be anisotropic. The result for isotropic materials can be derived directly from the anisotropic case. Following the procedure outlined in Suo [6], all the three sub-problems are solved analytically. The stress intensity factors computed from the stress-field are utilized to determine the driving force on the dislocations. For the sake of brevity, only the final results for the driving force on the dislocations are presented here and readers are referred to Yu et al. [7] for the complete analysis.

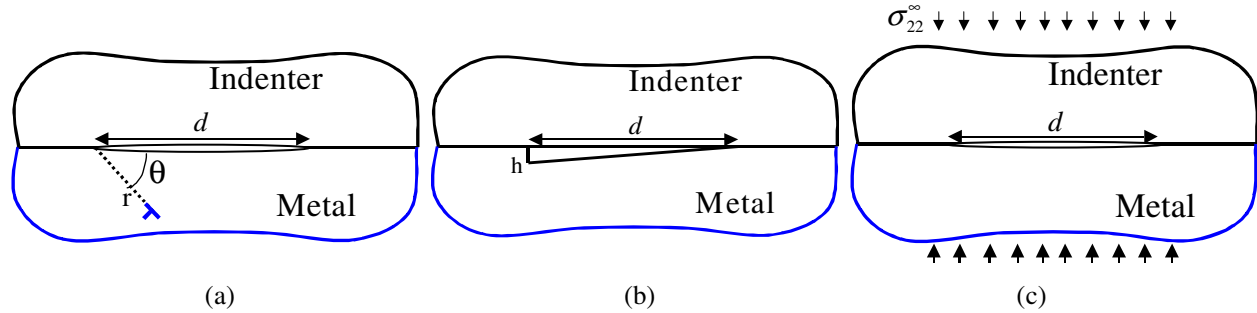


Figure 3 Decomposition of unit process model into three sub-problems

The configurational force on the dislocation emitted from the step is computed using conservation integrals. To illustrate the analytical solution, the driving force (J_D) on dislocations along three different slip planes at angles of $-\pi/4$, $-\pi/2$ and $-3\pi/4$ to the surface step are plotted in Fig. 4, as a function of distance (r) from the step. The non-dimensionalized parameters of the normal load, step height and interface adhesion used for computation are listed in the inset of Fig. 4. The positive driving force indicates that the dislocations are pushed away from the step and conversely, negative driving force implies attraction towards the step. At very large distances from the step, the remote normal loading dominates the driving force and consequently, the driving force plots for the three different orientations converge. At very short distances, the driving force is attractive and the attraction is weakest for the slip plane angle of $-\pi/2$ among the three angles considered. Thus, it is easier to nucleate dislocations along the $-\pi/2$ slip plane.

The dislocations emitted from the surface step attain an equilibrium position at distance (l) where the driving force becomes less than the Peierls resistance. The equilibrium positions for the dislocations along different slip planes are determined as a function of the applied normal load σ ($=\sigma_{22}^{\infty}$). The results for the dislocations along three different planes at $-\pi/4$, $-\pi/2$ and $-3\pi/4$ to the surface step are plotted in Fig. 5 (a), (b) and (c), for an adhesion Γ ($=\Gamma_{adh}$) and a step height indicated in the inset. The

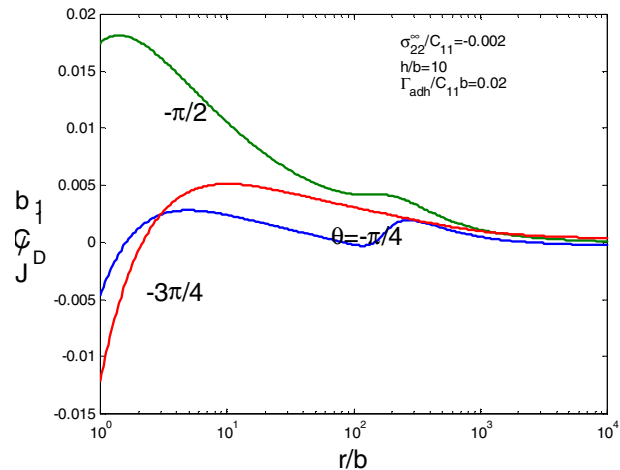


Figure 4 Driving force on a dislocation

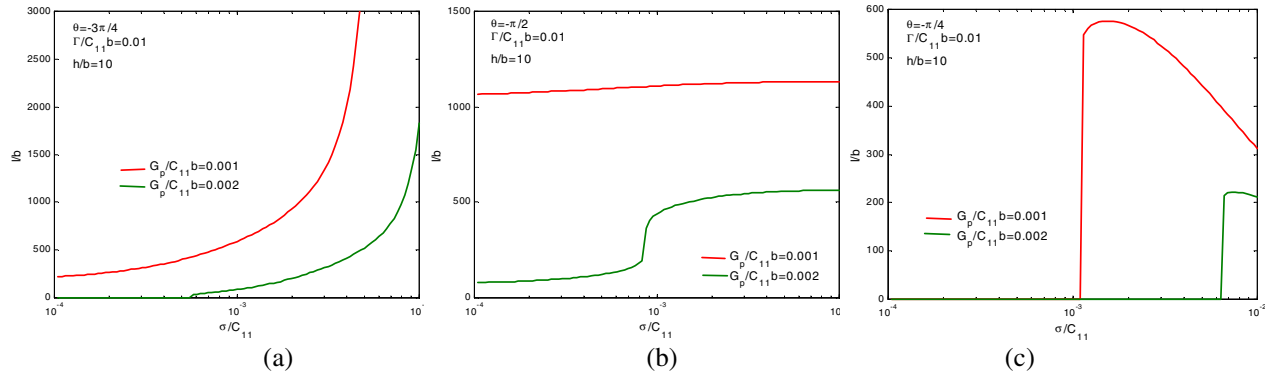


Figure 5 Equilibrium position of the dislocation along a slip plane

equilibrium positions along each plane are determined for two different Peierls stress (σ_p) values to study the influence of lattice resistance. Along the slip plane at $-\pi/4$, dislocation emission occurs only after the normal load becomes larger than a threshold value. Once emitted, the dislocation is pushed closer to the step as the load is increased. The dislocations along the slip plane at $-\pi/2$ are easily nucleated but remain at a fixed distance from the surface step as the contact load is increased. In contrast, along the slip plane at $-3\pi/4$ the distance of the dislocation from the surface step increases as the applied load is increased. The equilibrium positions of the dislocations clearly indicate that the dislocation nucleated from the surface step along different slip directions segregate into localized and bulk dislocations. Under the application of normal load, dislocations nucleated along the planes at $-\pi/4$ and $-\pi/2$ are localized near the surface step while the dislocations nucleated along plane at $-3\pi/4$ move away from the surface step into the bulk material. The former dislocation is named anti-load dislocation and the latter dislocation is called pro-load dislocation.

ATOMISTIC SIMULATIONS OF THE UNIT PROCESS MODEL

Atomistic simulations of stepped-surface contact were carried out to develop an understanding of dislocation nucleation processes and to calibrate the nucleation criterion used in the continuum analysis. The simulations were performed for a gold (Au) single crystal surface with surface steps, for which the crystallographic orientations and the geometry of the model are shown in Fig. 6. The bottom surface of the model is held fixed, while periodic boundary conditions are applied in both in-plane and out-of-plane lateral directions. The step height is composed of two atomic planes while the volume of the model contains approximately $80 \times 340 \times 5$ atoms.

The Au single crystal is modeled by embedded atom potential (EAM) developed by Foiles, Daw and Baskes [8]. Dislocation based continuum analysis indicates that surface adhesion plays an important role in the dislocation nucleation from the stepped surface. In order to investigate the influence of adhesion energy, three different types of indenters are utilized to

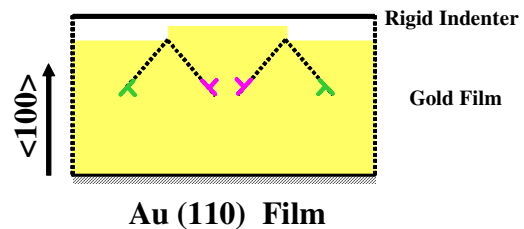


Figure 6 Schematic of the atomistic simulation

compress the stepped surface. As a limiting case of no adhesion energy, a layer of rigidly held gold atoms with only repulsive interaction is used to model a no-adhesion indenter. An indenter composed of rigidly held gold atoms with both attractive and repulsive potentials is made use of simulating the case of strong adhesion. The adhesion energy between the rigid gold surfaces along $\langle 100 \rangle$ direction is $\sim 0.92 \text{ Jm}^{-2}$ [8]. Modeling the indenter as a rigid graphite layer simulates the intermediate case of weak adhesion. A Lennard-Jones potential reported by Luedtke and Landman [9] is employed to model the interaction between the graphite and gold atoms. The adhesion energy between the graphite layer and the gold film is 0.12 Jm^{-2} .

The load-displacement curves obtained from the atomistic simulations of the three different indenters are plotted in Fig. 7. Varying the surface adhesion leads to three different regimes of instabilities, namely, just dislocation nucleation instability for no adhesive interaction, two distinct instabilities of surface adhesion and dislocation nucleation for weak adhesive interaction, and a simultaneous instability of surface adhesion and dislocation nucleation for strong adhesive interaction. The critical loads associated with dislocation nucleation for the three different surface adhesions are determined from the load-deflection curves. The continuum model was also utilized to compute the critical loads associated with the dislocation nucleation from the surface step along the easy guide directions of Au (110). For the computation, the Rice-Thomson parameter η is assumed to be equal to five times the burger vector of the nucleated dislocation and the critical loads are plotted as a function of step height in Fig. 8 for three different surface adhesion cases. The critical loads computed from the atomistic simulations are also plotted in Fig. 8. The comparison of the results clearly indicates that both atomistic simulations and continuum model predict that the critical loads associated with dislocation nucleation decreases with increasing surface adhesion energy. The results of the atomic simulations can also be used to determine the Rice-Thomson [6] parameter η used in the continuum model.

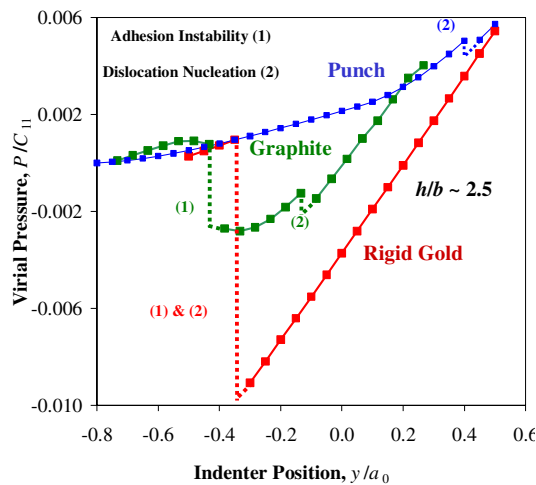


Figure 7 Load-deflection curves for atomistic simulation of unit-process model

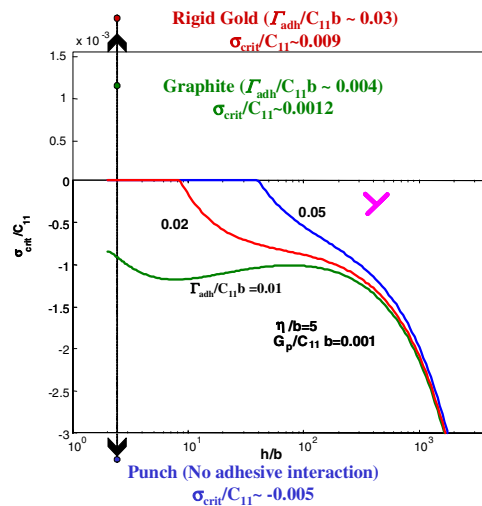


Figure 8 Comparison of dislocation nucleation load calculated from continuum model and atomistic simulation

DISCUSSION AND CONCLUDING REMARKS

A unit process model is analyzed under a multi-scale framework to study dislocation surface plasticity that explains the nano-meter scale surface roughness evolution during contact of surfaces. A continuum model is developed to study the dislocation nucleation from the surface step, while atomistic simulations are performed to determine the constitutive parameters used in the continuum analysis. The dislocation surface plasticity shows that the surface steps generate stress concentrations to nucleate dislocations near the surface step, and the geometry of the surface steps and the slip systems of easy glide segregate pro- and anti-load dislocations. The segregation is expected to induce a sub-micron thickness tensile-stress layer near the surface, and the tensile stress layer may accelerate nano-meter scale wear processes. The analyses also show significance of adhesion effects on nano-meter scale surface plasticity, indicating that plastically conforming adhesion can be induced by interface interaction only, without external loading, which may lead to cold welding. The atomistic simulations provide details of deformation-instability mechanisms depending on the strength of adhesion; such nano-meter scale instability mechanisms can explain various hierarchies of dissipative mechanisms in surface plasticity associated with surface adhesion. Atomistic simulations also show formation of Shockley partials and Lomer locks of the surface dislocations, indicating that further refined cooperative dislocation process model is needed for developing theory of meso-scale surface plasticity.

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