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Size dependence of energy storage and dissipation in a discrete dislocation plasticity analysis of static friction

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Abstract

The initiation of frictional sliding between a flat-bottomed indenter and a planar single crystal substrate is analyzed using discrete dislocation plasticity. Plastic deformation is modeled through the motion of edge dislocations in an elastic solid with the lattice resistance to dislocation motion, dislocation nucleation, dislocation interaction with obstacles and dislocation annihilation incorporated through a set of constitutive rules. The adhesion between the indenter and the substrate is modeled using a shear traction versus sliding displacement cohesive relation. The evolution of the energy storage and dissipation are calculated as a function of contact size.

Keywords: Dislocations; Mechanical properties; Friction; Plastic; Size effects; Computer simulation

1. Introduction

Frictional sliding is a complex process involving contact with multiple asperities, typically of a range of sizes. One issue is the magnitude of the friction force necessary to slide across a single asperity, $F_{\rm fr}$. Bowden and Tabor [1] developed a theory in which $F_{\rm fr}$ is taken to be proportional to the area of the contact $A_{\rm c}$ via

$$F_{\rm fr} = \tau_{\rm fr} A_{\rm c}. \qquad (1)$$

In this "plastic junction" theory of Bowden and Tabor [1] it is implicitly assumed that the friction stress $\tau_{\rm fr}$ is independent of the contact area. In [2], the initiation of sliding between a flat-bottomed indenter and a planar metallic single crystal substrate was analyzed using discrete dislocation plasticity. A range of contact sizes was found for which $\tau_{\rm fr}$ is size dependent. It was also found that the dislocation structure that accompanies sliding varied with the contact size.

A related issue of interest is the extent to which the plastic dissipation depends on contact size. The work expended in sliding is partitioned into the work required to overcome adhesion, the energy dissipated in plastic flow and the energy stored in the dislocation structure that develops. Here, the evolution of the energy partitioning is analyzed for three of the contact sizes in [2]. Each contact size considered exhibits qualitatively different behavior.

2. Method of analysis

Plane strain discrete dislocation analyses of the initiation of sliding between a perfectly flat indenter and a planar single crystal substrate are carried out as sketched in Fig. 1. For computational efficiency, the edge dislocations are confined to a region near the indenter as sketched in Fig. 1 and the computations are terminated before any dislocations reach the boundary of this region.

The dislocations are modeled as line singularities in an isotropic elastic solid. Consistent with the plane strain condition, only edge dislocations are considered, all having the

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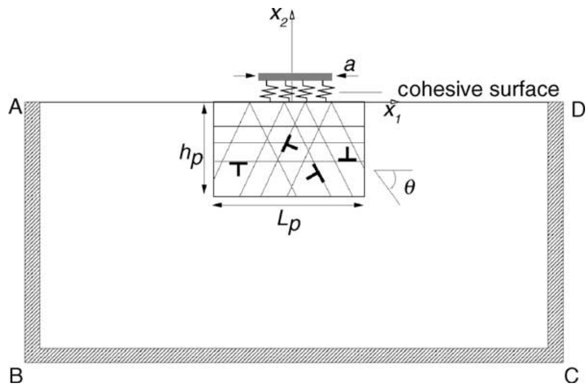

Fig. 1. Sketch of the boundary value problem considered.

same Burgers vector. Initially, the material is free of mobile dislocations and dislocations can be generated from randomly distributed discrete sources.

A cohesive surface is used to model the adhesion between the two contacting surfaces. In [2], two forms of the cohesive relation were considered. Here, attention is confined to the "non-softening" relation in [2] given by:

$$T_t = \begin{cases} -\tau_{max}\frac{\Delta_t}{\delta_t} & \text{if} \quad |\Delta_t| < \delta_t; \\ -\tau_{max}\text{sign}(\Delta_t) & \text{otherwise}, \end{cases} \tag{2}$$

where $\Delta_t = u_1(x_1, 0)$ is the tangential displacement jump across the cohesive surface, T_t the shear traction and τ_{max} and δ_t are prescribed constants.

A displacement, U, is imposed in the x_1 direction to simulate the relative sliding of the two contacting surfaces and attention is focused on the initiation of sliding. The computation of the deformation history is carried out in an incremental manner with U increased monotonically as described in [2] with superposition, [4], used to satisfy the boundary conditions. Dislocation rules are given for: (i) dislocation glide; (ii) annihilation; (iii) nucleation; and (iv) obstacle pinning.

From conservation of energy, the work done by the loading is

$$W = a\int_0^U \tau\, dU = \Phi + W_{plas} + W_{cohes} \tag{3}$$

where τ is the average contact shear stress, Φ the elastic energy stored in the material, W_{plas} is the plastic dissipation and W_{cohes} is the energy expended in the cohesive surface.

Recently, Benzerga et al. [5] have used discrete dislocation plasticity analyses to calculate the evolution of the stored energy of cold work and plastic dissipation and corresponding analyses are carried out here. The elastic energy stored in the material is obtained via

$$\Phi = \int_A \phi_e\, dA, \quad \phi_e = \frac{1}{2}\sigma_{ij}\epsilon^*_{ij} \tag{4}$$

where ϵ^*_{ij} is the elastic strain. Also, in calculating Φ a region of radius $4b$ is excluded around each dislocation core. Numerical checks showed that decreasing the core radius to $2b$ had a negligible effect on Φ, although the order of integration required to calculate Φ accurately then had to be increased.

Because in discrete dislocation plasticity, the plastic part of the deformation is associated with the evolution of displacement jumps across the slip planes, the displacement gradient field, needed to compute strains, involves delta functions. Here, an approximation is used to calculate the plastic dissipation. A smooth strain rate field, $\dot{\epsilon}^d_{ij}$, is introduced in each finite element that is computed by differentiating the total displacement rate field $\dot{u}_i$ in that element using the finite element shape functions. Then, at each point within an element, the plastic dissipation, W_{plas}, is the stress working through $\dot{\epsilon}^d_{ij}$ minus the energy stored. The total plastic dissipation is obtained by integrating over all elements so that

$$W_{plas} = \int_A w_{plas} dA, \quad w_{plas} = \int_0^t \sigma_{ij}\dot{\epsilon}^d_{ij} dt - \frac{1}{2}\sigma_{ij}\epsilon^*_{ij} \tag{5}$$

The cohesive energy, W_{cohes} at time t, is given by

$$W_{cohes} = \int_{S_{coh}} w_{cohes} dS, \tag{6}$$

where w_{cohes} is obtained as $\int T_t d\Delta_t$ where T_t and Δ_t are related by Eq. (2).

3. Results

The single crystal substrate is taken to have three slip systems: oriented at $\theta = \pm 60^\circ$ and $\theta = 0^\circ$ with respect to the contact surface $x_2 = 0$. Each slip system consists of equally placed slip planes $100b$ apart in the process window, where $b = 0.25$ nm is the magnitude of the Burgers vector. A density of sources, $\rho_{src} = 72\ \mu m^2$, distributed on each slip plane nucleate a dipole when the Peach-Koehler force exceeds a critical value of $\tau_{nuc}b$ during a period of time $t_{nuc} = 10$ ns; τ_{nuc} has a Gaussian distribution with mean $\bar{\tau}_{nuc} = 50$ MPa and standard deviation 10 MPa. There is also a density of obstacles, $\rho_{obs} = 124\ \mu m^2$, with obstacle strength $\tau_{obs} = 150$ MPa. The dislocation velocity is taken to be proportional to the Peach-Koehler force with drag coefficient $B = 10^{-4}$ Pa s and the annihilation distance is $6b$. The crystal elasticity is taken to be isotropic with $E = 70$ GPa and $\nu = 0.33$. The cohesive properties are given by $\tau_{max} = 300$ MPa and $\delta_t = 0.5$ nm.

The effect of the contact size a on the friction stress, τ_{fr}, was studied in [2]. It was found that the τ_{fr} versus a curve exhibits two plateaus: for large contacts ($a \geq 10\ \mu m$), τ_{fr} is of the order of the yield strength and essentially independent of a, while for small contacts ($a < 0.5\ \mu m$), $\tau_{fr} = \tau_{max}$. In the transition regime, $\tau_{fr} \propto a^{-1/2}$ as found on a different basis in [3].

The evolution of energy storage and dissipation is considered for three contact sizes; 10 μm, a contact size on the lower plateau; 1 μm, a transition contact size; and 0.1 μm, a contact size on the upper plateau ($\tau_{fr} = \tau_{max}$). On the lower plateau, plastic deformation is highly localized directly be-