AN ATOMISTIC VIEW OF INTERFACE SLIDING AND DISLOCATION PLASTICITY IN THIN FILMS

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ABSTRACT

Atomistic simulations are carried out to study the effect of atomic sliding capability at the interface between a plastically deforming film and a stiff substrate. Two dimensional molecular statics modeling is utilized to corroborate the overall film response and the nano-scale defect mechanisms. The numerical model consists of atoms of the metallic film having a close-packed crystal structure. The substrate is not explicitly included but special displacement constraint is imposed on the bottom boundary atoms, which are conceived to be the interface layer adjacent to the substrate. An intentional initial point defect is included in the model for triggering dislocation activities which result in a ductile film response. A free-sliding interface is shown to be able to cause ìreflectionî of oncoming dislocations and enhance film plasticity. A rigidly bonded interface, on the other hand, is seen to resist approaching dislocations. Partial sliding results in a transitional behavior between the two extremes, as revealed in our parametric analysis. The dislocation-interface reaction occurs more sluggishly as the atomic sliding capability decreases. The sliding capability of interface atoms is also seen to dictate the overall deformation and fracture behavior of the film.

1 INTRODUCTION

The atomistics of small-scale plasticity and the interaction of dislocations with the film-substrate interface are considered in this study. Our recent work has aimed at providing an atomic-scale picture on the interface-mediated plasticity in thin metal films [1]. Through two-dimensional (2D) molecular statics simulations it was shown that the elimination of a free surface facilitated by a stiff substrate enhances the yield strength of the film by restricting dislocation activities. In the present study, we extend the analysis to include the effect of controlled atomic sliding capability along the interface. The modeling also features an approximately 50% increase in film thickness compared to the precious study [1], with the purpose of examining salient features which may be affected by the problem size.

2 APPROACH

Figure 1 shows the model system, which is a close-packed planar crystal (containing 2276 atoms) with one of its close-packed directions parallel to the tensile loading (x) axis. To assist in triggering the onset of crystal plasticity, an artificial defect, in the form of a self-interstitial, is introduced in the model and allowed to equilibrate with its surrounding atoms before the loading steps commence. This technique enables ductile elastic-plastic behavior and the underlying atomistic processes to be simulated with the simple pair potential adopted here [2]. The Morse interatomic potential is used with the parameters determined by fitting to experimental data of the equilibrium lattice parameter, cohesive energy and bulk modulus of copper featuring near-neighbor interactions [3]. The molecular statics simulation of tensile stretching is carried out by prescribing a small displacement in the x direction on the right-hand boundary atoms at each step while fixing the x positions of the left-hand boundary atoms. In response to each loading step the atomic particles are allowed to iteratively reach their new equilibrium positions. The overall tensile load is calculated by summing the x-component force along the boundary atoms where displacements are prescribed. The bottom boundary atoms are conceived to be the interface layer with the substrate, with their motion in y-direction prohibited. No atoms are allowed to go below the interface.

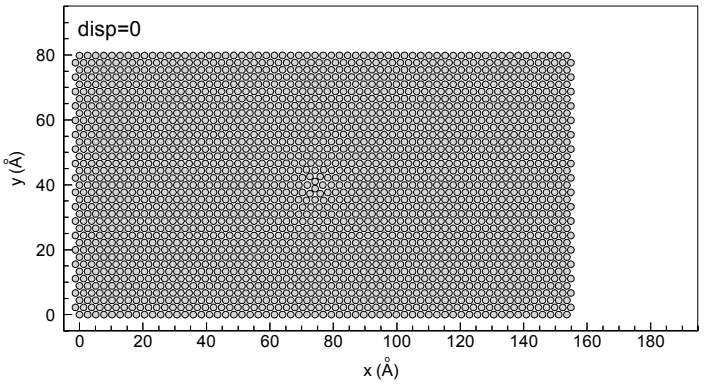

Figure 1: Initial atomic configuration for simulating the thin film (the substrate material is not specifically included). A self-interstitial is arbitrarily placed at near $x = 75 \approx$ and $y = 40 \approx$ and allowed to equilibrate with its surroundings before the loading simulation starts.

The interface sliding capability is facilitated by restricting the x-direction movement of interface atoms to various extents. In the extreme case of no slide, the x-component displacements of interface atoms are made proportional to the prescribed boundary displacement, simulating perfect bonding with the substrate *which controls the macroscopic deformation*. Different extents of sliding are controlled by allowing certain maximum x-component displacements of interface atoms. The maximum allowable displacement of each atom along the interface is expressed as

$$u_{x,\max} = k \cdot r_{\text{int}}, \tag{1}$$

where r_{int} represents the spacing between adjacent atoms along the interface at the beginning of the *current* loading increment (controlled by the prescribed boundary displacement), and k is the sliding parameter. The parameter k is henceforth used to designate the extent of sliding allowed in the model. The no-slide case corresponds to $k = 0$.

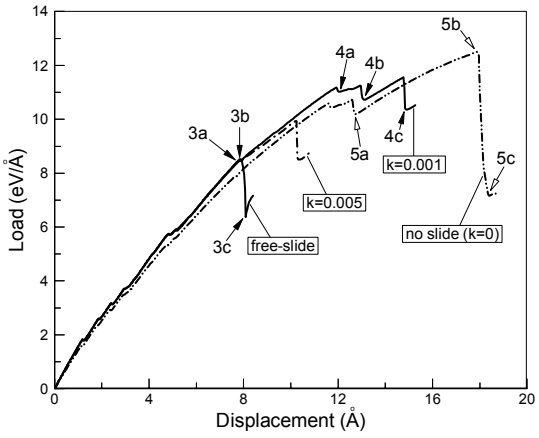

Figure 2: Overall tensile load-displacement curves obtained from the simulation. The interface sliding capabilities are denoted by the constant k. Select atomic snapshots corresponding to different stages of deformation are shown in Figs. 3-5 as labeled.

3 RESULTS AND DISCUSSION

Figure 2 shows the overall load-displacement curves of the films with various interface sliding capabilities. The curves are shown only up to their first significant load drop (chosen to be greater than 10% of the peak load), which signifies gross plastic yielding with at least one slip step created at the free surface (see below). There is a general trend that, as interface sliding becomes more difficult (decreasing k), the major load drop becomes more delayed. The symbols such as 3a, 3b etc. labeled along the curves in Fig. 2 indicate the figure numbers below, where the atomic snapshots during the deformation histories are shown.

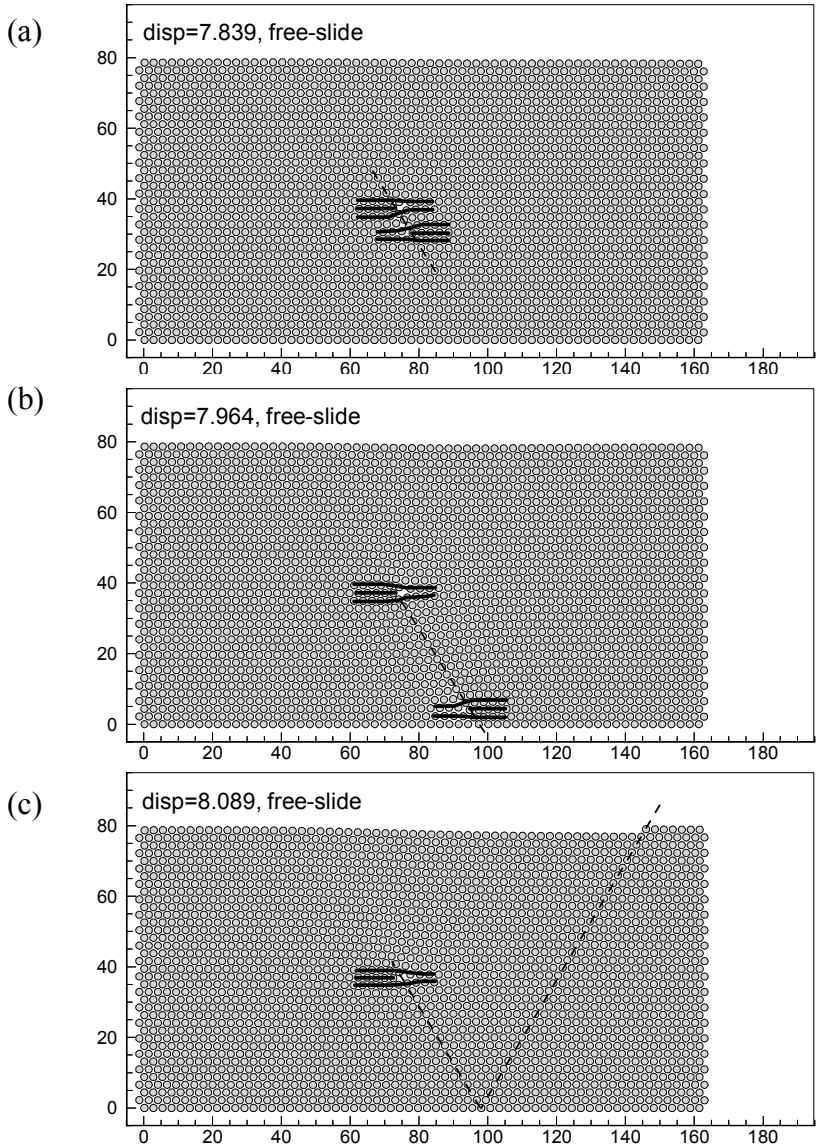

Figure 3: Snapshots of atomic configurations at points 3a, 3b and 3c labeled in Fig. 2 for the film with a free sliding capability.

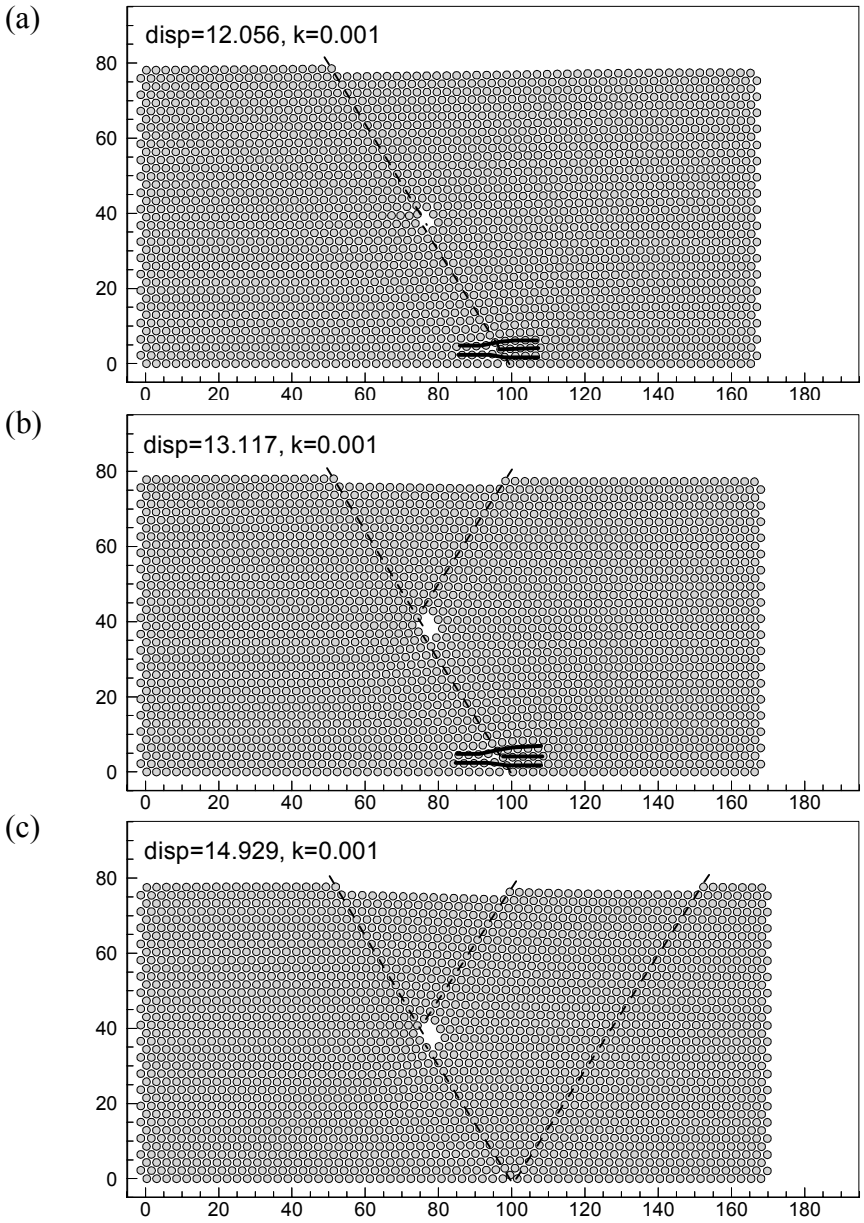

Figure 4: Snapshots of atomic configurations at points 4a, 4b and 4c labeled in Fig. 2 for the film with a sliding capability $k = 0.001$.

The snapshots presented in Figs. 3-5 are largely self-explanatory, so only minimal descriptions are given here for conserving space. In these figures dark lines connecting some atoms are used to highlight the dislocations in an elementary manner. The dashed lines indicate their slip paths. In Fig. 3(a), the initial point defect has evolved into a pair of dislocations in response to the macroscopic deformation. The lower dislocation has slipped to near the bottom

interface in Fig. 3(b) and has been ìreflectedî by the interface and slipped out of the crystal to create a slip step in Fig. 3(c). This process correlates with the large load drop observed in Fig. 2. The ìreflectedî dislocation, having a different Burgers vector from before the reflection, is in fact the outcome of dislocation reaction at the free-sliding interface as discussed in reference [1]. A qualitatively similar behavior was also observed in the case of k = 0.005. A notable difference (not shown here) is that, with a sliding limit imposed, the ability of the interface atoms to accommodate the oncoming dislocation is reduced so the dislocation-interface reaction is delayed (Fig. 2).

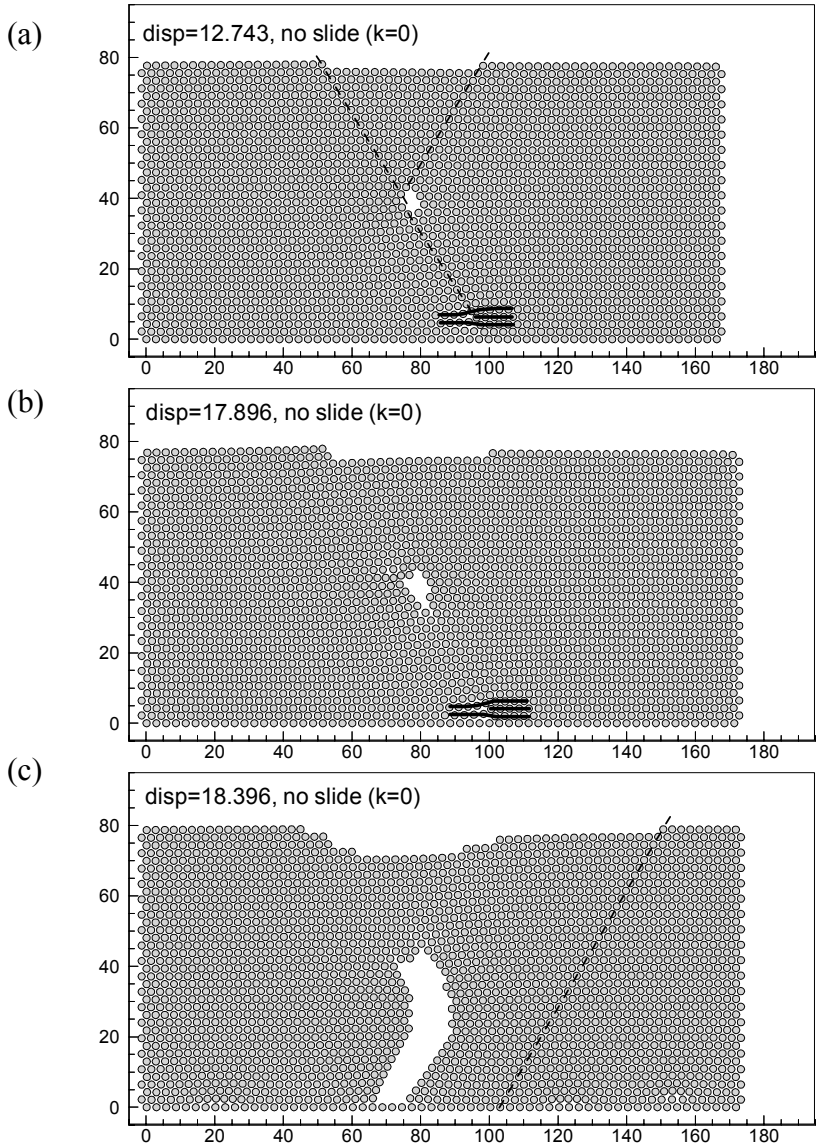

Figure 5: Snapshots of atomic configurations at points 5a, 5b and 5c labeled in Fig. 2 for the film with no sliding capability, k = 0.

When the sliding capability is further restricted (Figs. 4 and 5), a fundamental change in behavior can be seen. In the case of $k = 0.001$, the load reduction occurs in three successions (4a, 4b and 4c), each associated with the creation of a slip step. The dislocation reaction at the interface and the subsequent upward slip becomes more sluggish, resulting in the last load drop among the three. In addition, the reaction is imperfect because it left behind a local disturbance in atomic packing clearly visible at the interface (Fig. 4(c)). Further, a void was created near the initial upper dislocation site. In Fig. 5 where no interfacial sliding is allowed, the dislocation-interface reaction is further delayed. In fact, it occurs *after* a major internal damage in the crystal is formed. The oncoming dislocation stays pinned near the interface until very late in the deformation process. The effect of the ìreflectionî process on the overall load-displacement response is masked by the ductile fracture of the film. Final failure occurs as a result of slip-induced void growth toward the interface side (not the free surface side) of the film.

The fracture configuration in Fig. 5(c) can be compared with the case of a free-sliding interface as shown in Fig. 6. It is interesting to note that a free-sliding interface results in a somewhat more brittle form of local fracture. In both cases failure occurs earlier on the interface side rather than the free surface side of the film.

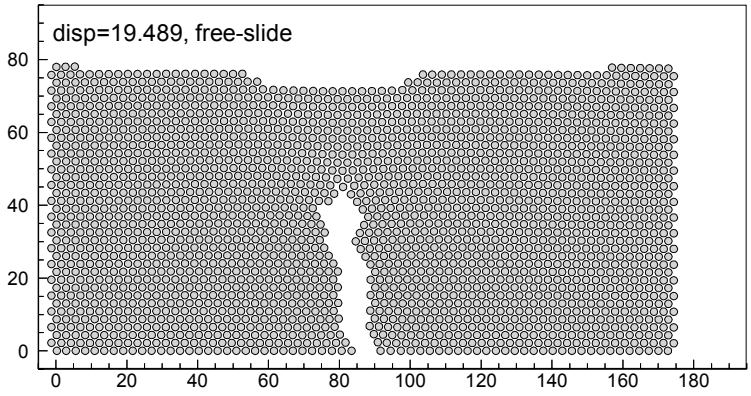

Figure 6: Snapshots of atomic configurations at near final fracture for the case of *free slide*.

4 CONCLUDING REMARKS

The present analyses help to provide some quantitative insight into the behavior of interface sliding at the atomic scale. The sliding parameter k used here to specify the maximum allowable sliding distance corresponds to exceedingly small local displacements. Nevertheless, the very small-scale sliding operation is still able to generate a very wide range of film response, implying the great sensitivity of thin-film plasticity to the atomistic characteristics at the interface.

5 REFERENCES

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[3] R. Phillips, *Crystals, Defects and Microstructures ñ Modeling Across Scales*, Cambridge University Press, 2001, p. 206.